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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	DEC 21	IPC search and display fields enhanced in CA/CAplus with the IPC reform
NEWS	4	DEC 23	New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/ USPAT2
NEWS	5	JAN 13	IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS	6	JAN 13	New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to INPADOC
NEWS	7	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS	8	JAN 17	IPC 8 in the WPI family of databases including WPIFV
NEWS	9	JAN 30	Saved answer limit increased
NEWS	10	JAN 31	Monthly current-awareness alert (SDI) frequency added to TULSA
NEWS	11	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS	12	FEB 22	Status of current WO (PCT) information on STN
NEWS	13	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS	14	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS	15	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	16	FEB 28	MEDLINE/LMEDLINE reload improves functionality
NEWS	17	FEB 28	TOXCENTER reloaded with enhancements
NEWS	18	FEB 28	REGISTRY/ZREGISTRY enhanced with more experimental spectral property data
NEWS	19	MAR 01	INSPEC reloaded and enhanced
NEWS	20	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS	21	MAR 08	X.25 communication option no longer available after June 2006
NEWS	22	MAR 22	EMBASE is now updated on a daily basis

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
http://download.cas.org/express/v8.0-Discover/

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* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:48:09 ON 30 MAR 2006

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:48:19 ON 30 MAR 2006
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 MAR 2006 HIGHEST RN 878378-71-3
DICTIONARY FILE UPDATES: 28 MAR 2006 HIGHEST RN 878378-71-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

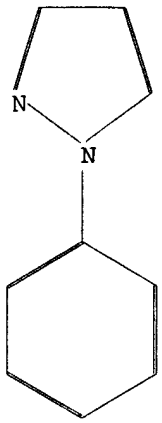
****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

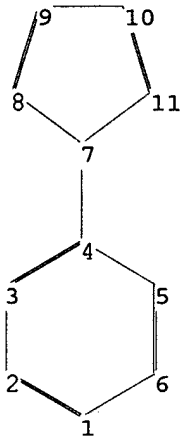
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10519356\Struc 1.str



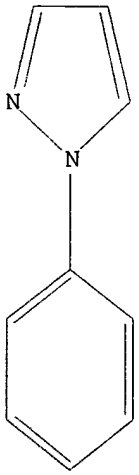


ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
4-7
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
4-7 7-8 7-11 8-9 9-10 10-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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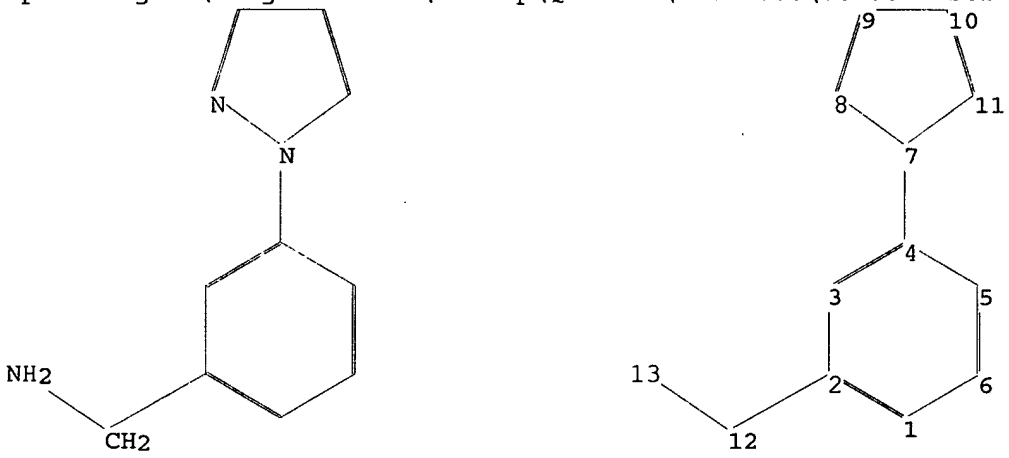
=> l1
SAMPLE SEARCH INITIATED 12:48:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    15800 TO ITERATE

 12.7% PROCESSED     2000 ITERATIONS                                  50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       308473 TO   323527
PROJECTED ANSWERS:          153293 TO   163969

L2           50 SEA SSS SAM L1

=>
Uploading C:\Program Files\Stnexp\Queries\10519356\Struc 2.str
```




```
chain nodes :
12  13
ring nodes :
1  2  3  4  5  6  7  8  9  10  11
chain bonds :
2-12  4-7  12-13
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-11  8-9  9-10  10-11
exact/norm bonds :
4-7  7-8  7-11  8-9  9-10  10-11
exact bonds :
2-12  12-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:CLASS  13:CLASS
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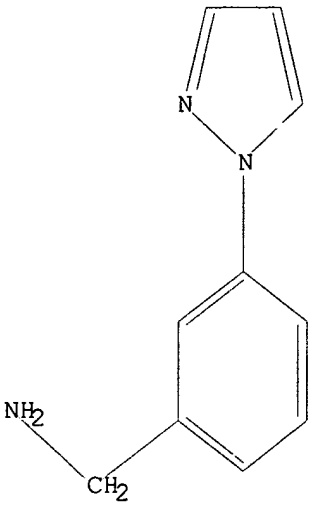
L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> l3
SAMPLE SEARCH INITIATED 12:49:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 557 TO ITERATE

100.0% PROCESSED 557 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 9725 TO 12555
PROJECTED ANSWERS: 9 TO 359

L4 9 SEA SSS SAM L3

=> l3 full
FULL SEARCH INITIATED 12:49:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 10980 TO ITERATE

100.0% PROCESSED 10980 ITERATIONS 167 ANSWERS
SEARCH TIME: 00.00.01

L5 167 SEA SSS FUL L3

=> file medline caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 167.38 167.59

FILE 'MEDLINE' ENTERED AT 12:49:44 ON 30 MAR 2006

FILE 'CAPLUS' ENTERED AT 12:49:44 ON 30 MAR 2006
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=> l5
L6 36 L5

=> dup rem l6
PROCESSING COMPLETED FOR L6
L7 36 DUP REM L6 (0 DUPLICATES REMOVED)

=> d ibib abs hitstr 1-36

L7 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1239173 CAPLUS
DOCUMENT NUMBER: 143:477963
TITLE: Preparation of pyrazolyl urea derivatives as TrkA kinase inhibitors useful in the treatment of cancer
INVENTOR(S): Lee, Wendy; Ladouceur, Gaetan; Dumas, Jacques; Smith, Roger; Ying, Shihong; Wang, Gan; Chen, Zhi; Liu, Qingjie; Mokdad, Holia Hatoum
PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA
SOURCE: PCT Int. Appl., 215 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005110994	A2	20051124	WO 2005-US15106	20050502
WO 2005110994	A3	20060202		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-566445P P 20040430
OTHER SOURCE(S): MARPAT 143:477963
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

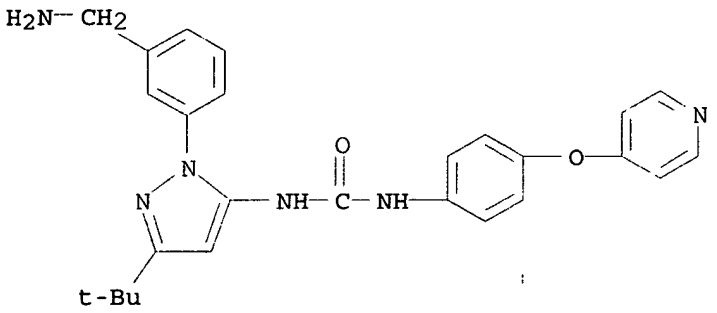
AB Title compds. I [R1-2 = H, alkyl, halo; A = Ph, pyridine, pyrimidine; B = phenylene, naphthylene; L = O, S, CH2; M = Ph, pyridine, pyrimidine; n =

0-1; X = O, SO2, etc.; Y = alkoxy, oxycarbonyl, amino, etc.] are prepared For instance, II is prepared from 4-[3-tert-butyl-5-[N'-[4-(pyridin-4-yloxy)phenyl]ureido]pyrazol-1-yl]benzoic acid Me ester (preparation given) and 2-(pyrrolidin-1-yl)ethylamine (DCE, AlMe3, 80°, 16 h). Compds. of the invention show significant inhibition of TrkA kinase (IC50 < 1 μM). I are useful for the treatment of cancer.

IT **869665-99-6P**, N-[1-[3-(Aminomethyl)phenyl]-3-tert-butyl-1H-pyrazol-5-yl]-N'-[4-(pyridin-4-yloxy)phenyl]urea **869666-00-2P**, N-[1-[3-(Aminomethyl)phenyl]-3-tert-butyl-1H-pyrazol-5-yl]-N'-[2-fluoro-4-[(2-methylpyridin-4-yl)oxy]phenyl]urea
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolyl urea derivs. as TrkA kinase inhibitors useful in treatment of cancer)

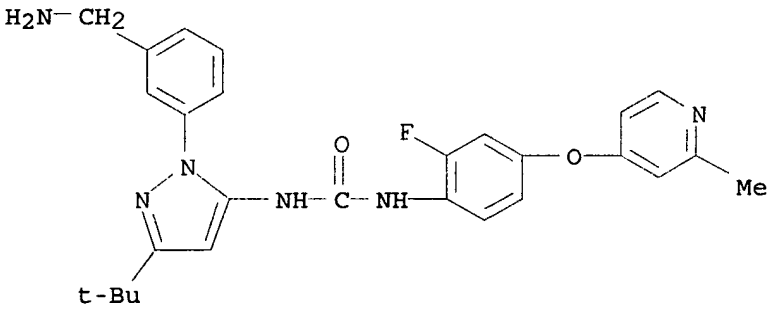
RN 869665-99-6 CAPLUS

CN Urea, N-[1-[3-(aminomethyl)phenyl]-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-[4-(4-pyridinyloxy)phenyl]- (9CI) (CA INDEX NAME)



RN 869666-00-2 CAPLUS

CN Urea, N-[1-[3-(aminomethyl)phenyl]-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-[2-fluoro-4-[(2-methyl-4-pyridinyl)oxy]phenyl]- (9CI) (CA INDEX NAME)



L7 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1103747 CAPLUS

DOCUMENT NUMBER: 143:387041

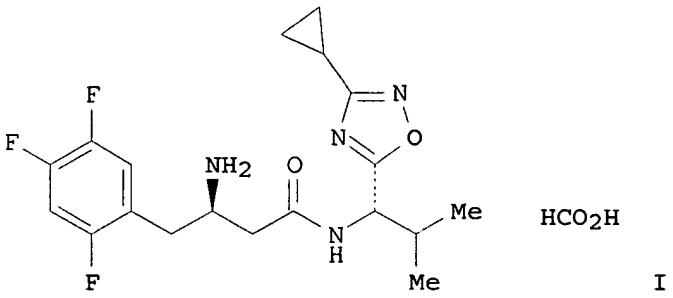
TITLE: Preparation of β-amino acid amides as dipeptidylpeptidase-IV (DPP-IV) inhibitors

INVENTOR(S): Edwards, Paul John; Feurer, Achim; Cerezo-Galves, Silvia; Matassa, Victor Giulio; Nordhoff, Sonja; Rosenbaum, Claudia; Bulat, Stephan

PATENT ASSIGNEE(S): Graffinity Pharmaceuticals A.-G., Germany
SOURCE: PCT Int. Appl., 150 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095343	A1	20051013	WO 2005-EP2010	20050225
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1593671	A1	20051109	EP 2004-5347	20040305
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				

PRIORITY APPLN. INFO.: EP 2004-5347 A 20040305
OTHER SOURCE(S): MARPAT 143:387041
GI

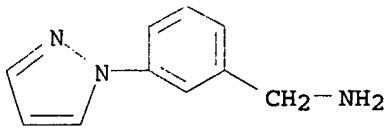


I

AB ZCR1R2CR3NH2CR4R5XNR6R7 [Z = (substituted) Ph, naphthyl, indenyl, indanyl, cycloalkyl, tetralinyl, decalinyl, heterocyclyl, heterobicyclyl; R1, R4 = H, F, OH, R4a; R2, R5 = H, F, R4b; R4a = (F-, Cl-substituted) alkyl, alkoxy; R4b = (F-, Cl-substituted) alkyl; R3 = H, alkyl; R1R2, R2R3, R3R4, R4R5 = atoms to form a (substituted) C3-7 cycloalkyl ring; X = SO, SO2, CO, CR13R14; R13, R14 = H, F, alkyl, etc.; R6, R7 = H, (CR29R30)mX1Z1, (substituted) alkyl, etc.; R29, R30 = H, halo, cyano, OH, NH2, CO2H, CONH2, SONH2, etc.; m = 0-4; X1 = bond, alkylene, alkyleneoxy, alkyleneimino, CO, etc.; Z1 = H, (substituted) alkyl, etc.], were prepared Thus, title compound (I) (multistep preparation given) inhibited DPP-IV with IC50 <100 nM.

IT **687635-04-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of amino acid amides as dipeptidylpeptidase-IV inhibitors)
RN 687635-04-7 CAPLUS
CN Benzenemethanamine, 3-(1H-pyrazol-1-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1021642 CAPLUS
DOCUMENT NUMBER: 143:311996
TITLE: Methods for inhibiting platelet activation and aggregation, and therapeutic uses for conditions or surgical procedures that may result in unwanted platelet aggregation
INVENTOR(S): Porter, Stephen R.; Flaharty, Kristen K.; Tcheng, James E.; Ferkany, John W.
PATENT ASSIGNEE(S): Vddi Pharmaceuticals, USA
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005087266	A1	20050922	WO 2005-US7440	20050307

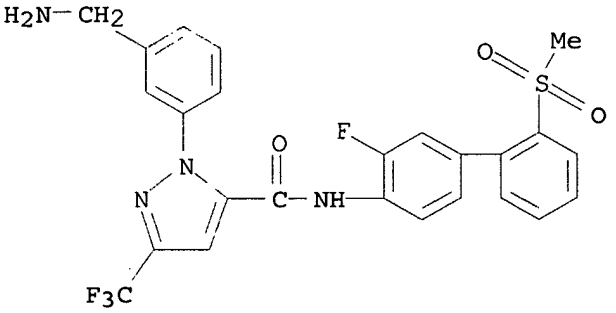
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-550792P P 20040305

AB The invention features methods for preventing platelet activation and aggregation and for treating individuals suffering from conditions or undergoing procedures that may result in unwanted platelet aggregation. The methods are based on the i.v., s.c., or transdermal administration of a platelet activation or aggregation inhibitor, e.g., xemilofiban, followed by oral administration of the same or a different platelet activation or aggregation inhibitor. The treatment may commence prior to a medical or surgical procedure or after the outbreak of an adverse medical condition, either of which results in the activation of platelets that may lead to thrombus formation, and may continue thereafter.

IT **292135-59-2**, DPC423
RL: ANT (Analyte); ANST (Analytical study)

(combination therapy for inhibition of platelet aggregation)
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1346235 CAPLUS
DOCUMENT NUMBER: 144:88279
TITLE: Preparation of 1-pyrazolyl-3-phenylurea p38 MAP kinase inhibitors as antiinflammatory medicaments
INVENTOR(S): Flynn, Daniel L.; Petillo, Peter A.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 214 pp., Cont.-in-part of U.S. Ser. No. 746,460.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005288286	A1	20051229	US 2004-886329	20040706
US 2004180906	A1	20040916	US 2003-746460	20031224
WO 2006014290	A2	20060209	WO 2005-US23100	20050630

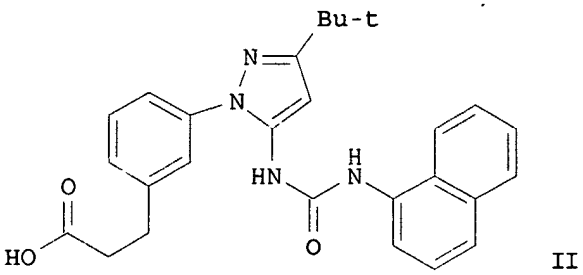
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2003-746460 A2 20031224

US 2002-437304P P 20021231
US 2002-437403P P 20021231
US 2002-437415P P 20021231
US 2002-437487P P 20021231
US 2004-886329 A 20040706

OTHER SOURCE(S): MARPAT 144:88279

GI



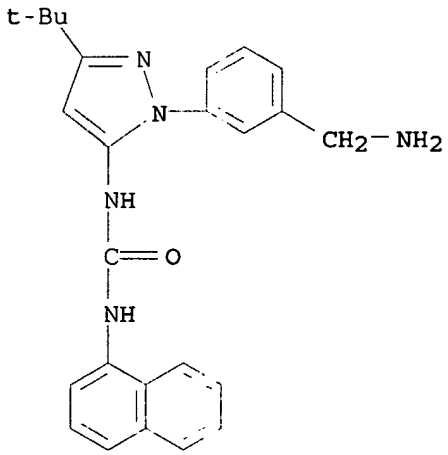
II

AB Title compds. (R1Xj)mA(NH)pLn(NH)pDEqYtQ [I; wherein R1 = (un)substituted (hetero)aryl; X, Y = independently O, S, NR6, NR6SO2, NR6CO, alkynyl, alkenyl, alkylene, O(CH2)h, NR6(CH2)h, wherein for each alkylene, O(CH2)h, and NR6(CH2)h, one of the methylene groups may be substituted with CO; h = 1-4; A = (un)substituted aryl, hetero(bi)cyclyl; D = (un)substituted Ph, pyrazolyl, pyrrolyl, imidazolyl, oxazolyl, thiazolyl, furyl, pyridyl, pyrimidyl; E = (un)substituted Ph, pyridinyl, pyrimidinyl; L = CO, SO2; j, m, n, p, q, t = independently 0, 1; Q = (un)substituted heterocyclyl, Ph, etc.; R6 = independently H, alkyl, allyl, TMS(CH2)2; with exceptions] were prepared as p38 MAP kinase inhibitors. In a preferred embodiment, modulation of the activation state of p38 kinase protein comprises the step of contacting the α-C helix, the α-D helix, the catalytic loop, the switch control ligand sequence, or the C-lobe residues of the kinase protein with I (no data). Although the methods of preparation are not claimed, prepns. and/or characterization data for .apprx.150 examples of I and many intermediates are included. For example, hydrogenation of 3-(3-aminophenyl)acrylic acid Me ester using 10% Pd/C in EtOH provided the propionate, which was treated with NaNO2 in the presence of 6N HCl and SnCl2•2H2O to give the hydrazine. Reaction of the hydrazine with 4,4-dimethyl-3-oxopentanenitrile in EtOH and 6N HCl afforded Me 3-[3-(3-tert-butyl-5-amino-1H-pyrazole-1-yl)phenyl]propionate. Coupling of the amine with 1-naphthyl isocyanate in CH2Cl2, followed by reduction with LiOH in THF/MeOH/H2O provided the urea II. In a competition assay with SKF 86002 as a fluorescent probe, the latter inhibited p38 MAP kinase with IC50 of 45 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of a wide variety of inflammatory conditions (no data).

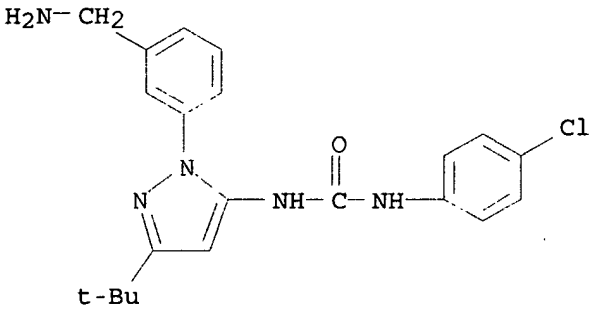
IT **725686-04-4P**, 1-[3-tert-Butyl-1-[3-(aminomethyl)phenyl]-1H-pyrazol-5-yl]-3-(naphthalen-1-yl)urea **725686-05-5P**, 1-[3-tert-Butyl-1-[3-(aminomethyl)phenyl]-1H-pyrazol-5-yl]-3-(4-chlorophenyl)urea
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (pyrazolyl)(aryl)urea p38 kinase inhibitors as antiinflammatory agents)

RN 725686-04-4 CAPLUS

CN Urea, N-[1-[3-(aminomethyl)phenyl]-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)



RN 725686-05-5 CAPLUS
CN Urea, N-[1-[3-(aminomethyl)phenyl]-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

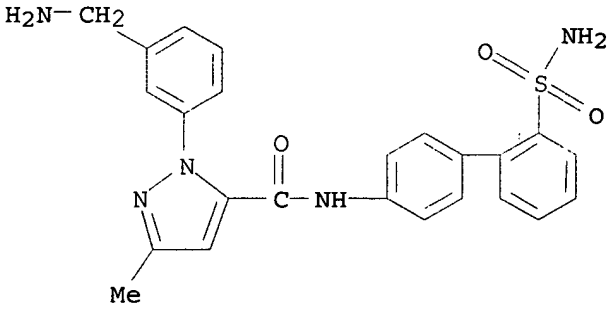


L7 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:511199 CAPLUS
DOCUMENT NUMBER: 143:145801
TITLE: Ligand-based assessment of factor Xa binding site flexibility via elaborate pharmacophore exploration and genetic algorithm-based QSAR modeling
AUTHOR(S): Taha, Mutasem O.; Qandil, Amjad M.; Zaki, Dhia D.; AlDamen, Murad A.
CORPORATE SOURCE: Faculty of Pharmacy, Department of Pharmaceutical Sciences, University of Jordan, Amman, Jordan
SOURCE: European Journal of Medicinal Chemistry (2005), 40(7), 701-727
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The flexibility of activated factor X (fXa) binding site was assessed employing ligand-based pharmacophore modeling combined with genetic algorithm (GA)-based QSAR modeling. Four training subsets of wide structural diversity were selected from a total of 199 direct fXa inhibitors and were employed to generate different fXa pharmacophoric hypotheses using CATALYST software over two subsequent stages. In the first stage, high quality binding models (hypotheses) were identified.

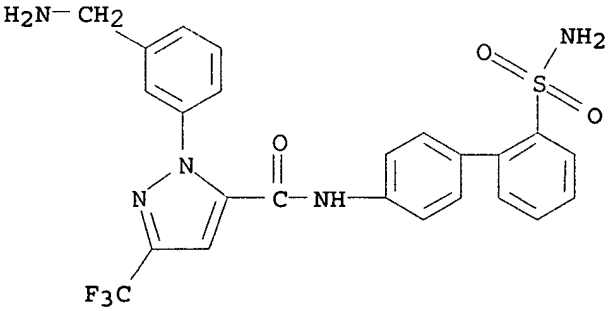
However, in the second stage, these models were refined by applying variable feature weight anal. to assess the relative significance of their features in the ligand-target affinity. The binding models were validated according to their coverage (capacity as a three-dimensional (3D) database search queries) and predictive potential as three-dimensional quant. structure-activity relationship (3D-QSAR) models. Subsequently, GA and multiple linear regression (MLR) anal. were employed to construct different QSAR models from high quality pharmacophores and explore the statistical significance of combination models in explaining bioactivity variations across 199 fXa inhibitors. Three orthogonal pharmacophoric models emerged in the optimal QSAR equation suggesting they represent three binding modes accessible to ligands in the binding pocket within fXa.

IT **209955-58-8 209955-60-2 209957-35-7 209957-47-1**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ligand-based assessment of factor Xa binding site flexibility via elaborate pharmacophore exploration and genetic algorithm-based QSAR modeling)

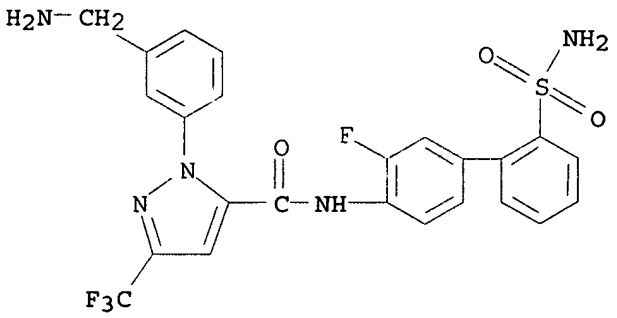
RN 209955-58-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



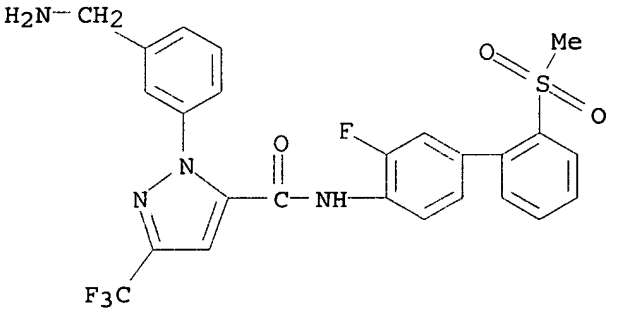
RN 209955-60-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:799558 CAPLUS
DOCUMENT NUMBER: 141:296012
TITLE: Preparation of factor Xa- and thrombin-inhibiting substituted benzamidines and sulfonylbenzamidines as potential anticoagulants
INVENTOR(S): Pinto, Donald J.; Qiao, Jennifer X.; Gangor, Timur; Lam, Patrick Y. S.; Li, Yun-long
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 279 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004083174	A2	20040930	WO 2004-US8033	20040317
WO 2004083174	A3	20041125		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
TD, TG

US 2004209863	A1	20041021	US 2004-801518		20040316
EP 1603562	A2	20051214	EP 2004-757516		20040317
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK					
PRIORITY APPLN. INFO.:			US 2003-455709P	P	20030318
			US 2004-801518	A	20040316
			WO 2004-US8033	W	20040317

OTHER SOURCE(S): MARPAT 141:296012
GI

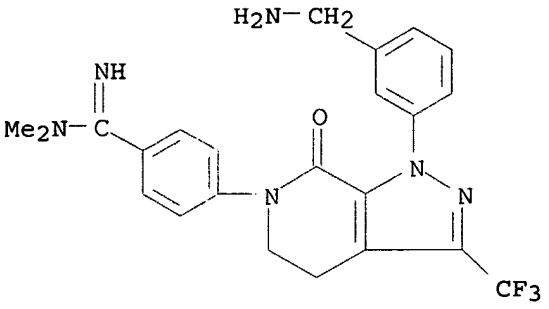
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. P4-M-M4 (I) [M = (un)substituted 3-10 membered carbocyclic or a 4-10 membered heterocyclic ring containing 1-3 O, N, or S atoms, alone or fused to an (un)substituted 5-7 membered carbocycle or heterocycle; P4 = Z-A-B; M4 = G-G1; A = (un)substituted 3-10 membered carbocyclic or 5-12 membered heterocyclic ring ; B = (un)substituted amidino, guanidino, iminomethyl; G = five or six-membered carbocycle or heterocycle fused to a benzene, pyridine, pyrimidine, pyrazine, or pyridazine ring; G1 = bond, (un)substituted alkyl, alkenyl, alkynyl; Z = (un)substituted alkylene], such as tetrahydropyrazolo[3,4-c]pyridinone II or (pyridinylaminocarbonylphenylaminocarbonyl)benzamidine III are prepared as inhibitors of Factor Xa and thrombin for use as anticoagulants. Deprotonation of 2-amino-4-chloropyridine and addition to 5-chloroisatoic anhydride yields N-(5-chloro-2-pyridinyl) 2-amino-5-chlorobenzamide (IV). Acid-mediated addition of dimethylamine to the nitrile of Me 4-cyanobenzoate, mesylation of the amidine nitrogen, and base-mediated hydrolysis of the ester yields 4-(N,N-dimethyl-N'-methylsulfonylamidino)benzoic acid (V). Coupling of IV and V mediated by BOP yields III. Some compds. of the invention inhibit human factor Xa with Ki values of ≤ 10 μM; in addition, some of the invention compds. inhibit thrombin in vitro. (no data).

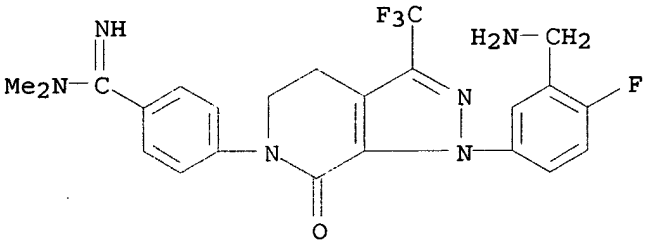
IT **764659-23-6P 764659-25-8P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of factor Xa- and thrombin-inhibiting substituted benzamidines and sulfonylbenzamidines as potential anticoagulants)

RN 764659-23-6 CAPLUS

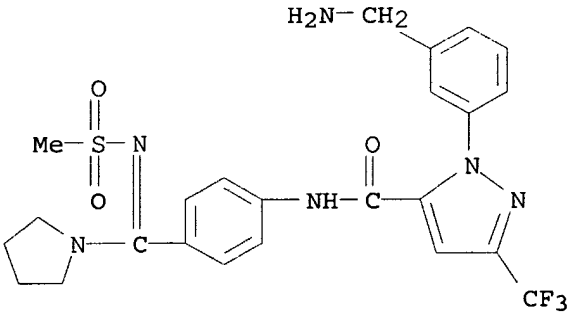
CN Benzenecarboximidamide, 4-[1-[3-(aminomethyl)phenyl]-1,4,5,7-tetrahydro-7-oxo-3-(trifluoromethyl)-6H-pyrazolo[3,4-c]pyridin-6-yl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



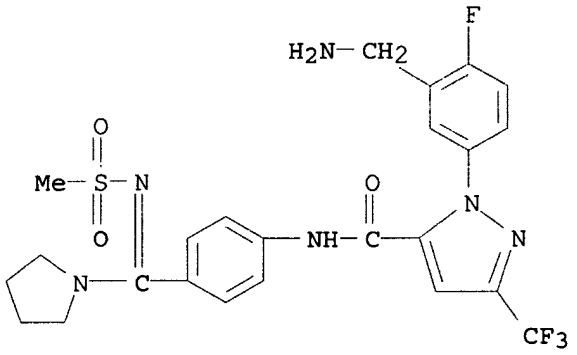
RN 764659-25-8 CAPLUS
CN Benzenecarboximidamide, 4-[1-[3-(aminomethyl)-4-fluorophenyl]-1,4,5,7-tetrahydro-7-oxo-3-(trifluoromethyl)-6H-pyrazolo[3,4-c]pyridin-6-yl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



IT **764658-97-1P 764658-98-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of factor Xa- and thrombin-inhibiting substituted benzamidines and sulfonylbenzamidines as potential anticoagulants)
RN 764658-97-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[[(methylsulfonyl)imino]-1-pyrrolidinylmethyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 764658-98-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[4-[[(methylsulfonyl)imino]-1-pyrrolidinylmethyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



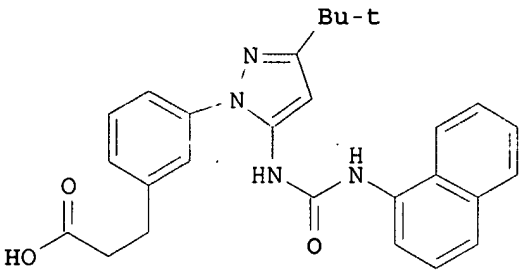
L7 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:589376 CAPLUS
DOCUMENT NUMBER: 141:140433
TITLE: Preparation of 1-pyrazolyl-3-phenylurea p38 MAP kinase inhibitors as antiinflammatory medicaments
INVENTOR(S): Flynn, Daniel L.; Petrillo, Peter A.
PATENT ASSIGNEE(S): Deciphera Pharmaceuticals, Inc., USA; Deciphera Pharmaceuticals, LLC
SOURCE: PCT Int. Appl., 207 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004060306	A2	20040722	WO 2003-US41449	20031226
WO 2004060306	A3	20050728		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004180906	A1	20040916	US 2003-746460	20031224
CA 2513627	AA	20040722	CA 2003-2513627	20031226
EP 1585734	A2	20051019	EP 2003-808576	20031226
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.:		
US 2002-437304P	P	20021231
US 2002-437403P	P	20021231
US 2002-437415P	P	20021231
US 2002-437487P	P	20021231
US 2003-463804P	P	20030418
US 2003-746460	A	20031224
WO 2003-US41449	W	20031226

OTHER SOURCE(S): MARPAT 141:140433

GI



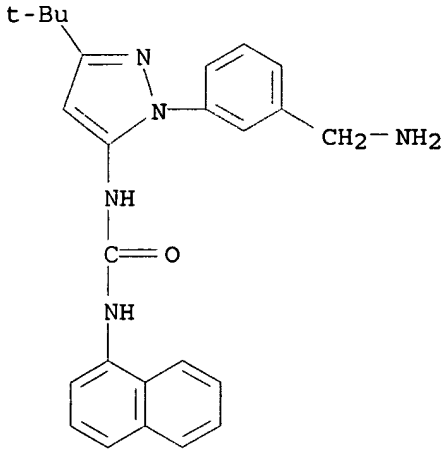
II

AB Title compds. (R1Xj)mA(NH)pLn(NH)pDEqYtQ [I; wherein R1 = (un)substituted (hetero)aryl; X, Y = independently O, S, NR6, NR6SO2, NR6CO, alkynyl, alkenyl, alkylene, O(CH2)h, NR6(CH2)h, wherein for each alkylene, O(CH2)h, and NR6(CH2)h, one of the methylene groups may be substituted with CO; h = 1-4; A = (un)substituted aryl, hetero(bi)cyclyl; D = (un)substituted Ph, pyrazolyl, pyrrolyl, imidazolyl, oxazolyl, thiazolyl, furyl, pyridyl, pyrimidyl; E = (un)substituted Ph, pyridinyl, pyrimidinyl; L = CO, SO2; j, m, n, p, q, t = independently 0, 1; Q = (un)substituted heterocyclyl, Ph, etc.; R6 = independently H, alkyl, allyl, TMS(CH2)2; with exceptions] were prepared as p38 MAP kinase inhibitors. In a preferred embodiment, modulation of the activation state of p38 kinase protein comprises the step of contacting the α-C helix, the α-D helix, the catalytic loop, the switch control ligand sequence, or the C-lobe residues of the kinase protein with I (no data). For example, hydrogenation of 3-(3-aminophenyl)acrylic acid Me ester using 10% Pd/C in EtOH provided the propionate, which was treated with NaNO2 in the presence of 6N HCl and SnCl2•2H2O to give the hydrazine. Reaction of the hydrazine with 4,4-dimethyl-3-oxopentanenitrile in EtOH and 6N HCl afforded Me 3-[3-(3-tert-butyl-5-amino-1H-pyrazole-1-yl)phenyl]propionate. Coupling of the amine with 1-naphthyl isocyanate in CH2Cl2, followed by reduction with LiOH in THF/MeOH/H2O provided the urea II. In a competition assay with SKF 86002 as a fluorescent probe, the latter inhibited p38 MAP kinase with IC50 of 45 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of a wide variety of inflammatory conditions (no data).

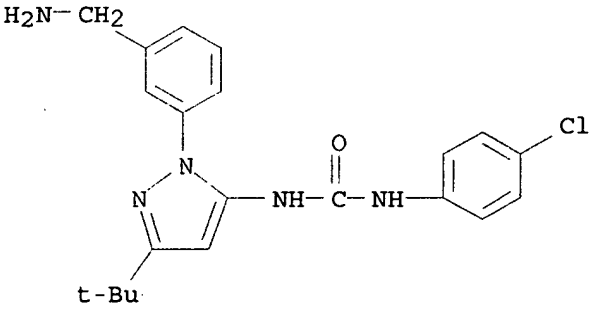
IT **725686-04-4P**, 1-[3-tert-Butyl-1-[3-(aminomethyl)phenyl]-1H-pyrazol-5-yl]-3-(naphthalen-1-yl)urea **725686-05-5P**, 1-[3-tert-Butyl-1-[3-(aminomethyl)phenyl]-1H-pyrazol-5-yl]-3-(4-chlorophenyl)urea
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (pyrazolyl)(aryl)urea p38 kinase inhibitors as antiinflammatory agents)

RN 725686-04-4 CAPLUS

CN Urea, N-[1-[3-(aminomethyl)phenyl]-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)



RN 725686-05-5 CAPLUS
CN Urea, N-[1-[3-(aminomethyl)phenyl]-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



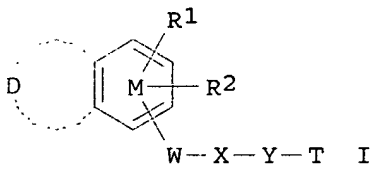
L7 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:20490 CAPLUS
DOCUMENT NUMBER: 140:77148
TITLE: Preparation of N-[4-(thiooxoheterocyclyl)phenyl]-2-phenyl-2H-pyrazole-3-carboxamides and corresponding imino-heterocyclyl derivatives as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis
INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner; Tsaklakidis, Christos; Gleitz, Johannes; Barnes, Christopher
PATENT ASSIGNEE(S): Merck Patent Gmbh, Germany
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004002477	A1	20040108	WO 2003-EP5898	20030605

WO 2004002477 C1 20040415
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

DE 10229070	A1	20040115	DE 2002-10229070		20020628
CA 2491271	AA	20040108	CA 2003-2491271		20030605
AU 2003238475	A1	20040119	AU 2003-238475		20030605
EP 1517685	A1	20050330	EP 2003-732540		20030605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
JP 2005535630	T2	20051124	JP 2004-516575		20030605
US 2005203127	A1	20050915	US 2004-519356		20041228
PRIORITY APPLN. INFO.:			DE 2002-10229070	A	20020628
			WO 2003-EP5898	W	20030605

OTHER SOURCE(S): MARPAT 140:77148
GI



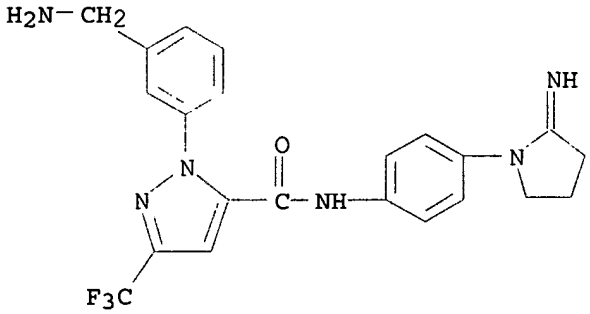
I

AB Title compds. [I; D = (N-, O-, S-interrupted) (substituted) C3-4 alkylene; M = Ph, aromatic heterocyclyl; R1, R2 = H, halo, (branched) (interrupted) (substituted) alkyl, NO2, cyano, OR3, N(R3)2, CO2R3, CON(R3)2, C(:S)N(R3)2, etc.; R3 = H, (branched) (interrupted) (substituted) alkyl, etc.; W = (substituted) (bi)cyclic aromatic (hetero)cyclyl; X = CONR3, CONR3C(R4)2, C(R4)2NR3, etc.; R4 = H, (branched) (interrupted) (substituted) alkyl; Y = alkylene, cycloalkylene, heterodiyl, aryldiyl; T = (substituted) (bi)cyclic aromatic heterocyclyl], were prepared Thus, 333 mg (3-[5-(4-[2-iminopyrrolidin-1-yl]phenylcarbamoyl)-3-trifluoromethylpyrazol-1-yl]benzyl)carbamic acid tert-Bu ester (preparation given) in EtOH was treated with HCl in ether to give 289 mg N-[4-(2-iminopyrrolidin-1-yl)phenyl]-1-(3-aminomethylphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide. The latter gave affinity to the receptor Xa with IC50 = 9,6·10-9 M and to the receptor VIIa with IC50 = 2,3·10-8 M.

IT **640287-97-4P 640288-21-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

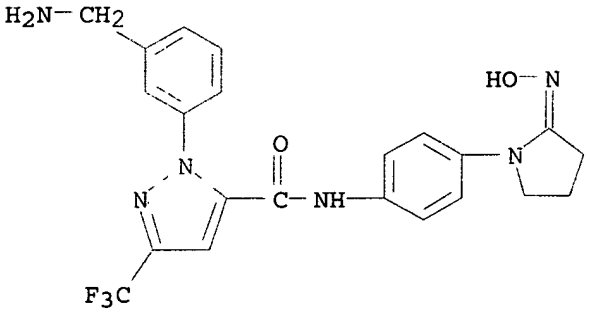
RN 640287-97-4 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

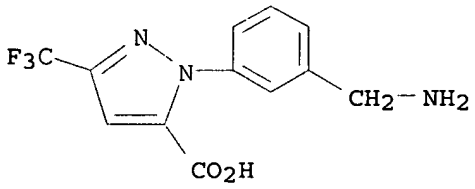


●2 HCl

RN 640288-21-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[2-(hydroxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

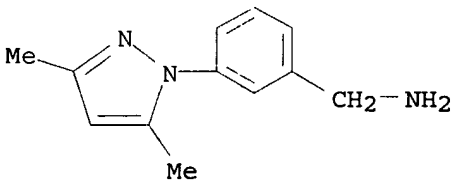


IT **640287-98-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)
RN 640287-98-5 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:673254 CAPLUS
DOCUMENT NUMBER: 142:197981
TITLE: Copper-diamine-catalyzed N-arylation of pyrroles, pyrazoles, indazoles, imidazoles, and triazoles. [Erratum to document cited in CA141:207140]
AUTHOR(S): Antilla, Jon C.; Baskin, Jeremy M.; Barder, Timothy E.; Buchwald, Stephen L.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Journal of Organic Chemistry (2004), 69(19), 6514
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB On page 5578, an important reference describing the copper-catalyzed N-arylation of pyrazoles was left out of the manuscript: Cristau, H.-J., Cellier, P. P.; Spindler, J.-F.; Taillefer, M. Eur. J. Organic Chemical 2004, 695-709.
IT **741717-65-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of N-arylpyrroles, -pyrazoles, -indazoles, -imidazoles, and -triazoles via copper-diamine-catalyzed N-arylation of pyrroles, pyrazoles, indazoles, imidazoles, or triazoles with aryl halides (Erratum))
RN 741717-65-7 CAPLUS
CN Benzenemethanamine, 3-(3,5-dimethyl-1H-pyrazol-1-yl)- (9CI) (CA INDEX NAME)



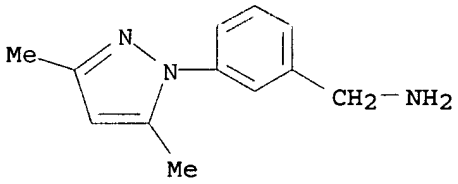
L7 ANSWER 10 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:553595 CAPLUS
DOCUMENT NUMBER: 141:207140
TITLE: Copper-diamine-catalyzed N-arylation of pyrroles, pyrazoles, indazoles, imidazoles, and triazoles
AUTHOR(S): Antilla, Jon C.; Baskin, Jeremy M.; Barder, Timothy E.; Buchwald, Stephen L.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Journal of Organic Chemistry (2004), 69(17), 5578-5587
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:207140
AB A copper-catalyzed N-arylation reaction of π-excessive nitrogen heterocycles is presented. The coupling of either aryl iodides or aryl bromides with common nitrogen heterocycles (pyrroles, pyrazoles, indazoles, imidazoles, and triazoles) was successfully performed in good yield with catalysts derived from diamine ligands and CuI. General

conditions that tolerate functional groups such as aldehydes, ketones, alcs., primary amines, and nitriles on the aryl halide or heterocycle, were found. Hindered aryl halides or heterocycles were also found to be suitable substrates using the conditions reported herein.

IT **741717-65-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of N-arylpyrroles, -pyrazoles, -indazoles, -imidazoles, and -triazoles via copper-diamine-catalyzed N-arylation of pyrroles, pyrazoles, indazoles, imidazoles, or triazoles with aryl halides)

RN 741717-65-7 CAPLUS

CN Benzenemethanamine, 3-(3,5-dimethyl-1H-pyrazol-1-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 11 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1151496 CAPLUS

DOCUMENT NUMBER: 142:328858

TITLE: The chimpanzee (Pan troglodytes) as a pharmacokinetic model for selection of drug candidates: Model characterization and application

AUTHOR(S): Wong, Harvey; Grossman, Scott J.; Bai, Stephen A.; Diamond, Sharon; Wright, Matthew R.; Grace, James E., Jr.; Qian, Mingxin; He, Kan; Yeleswaram, Krishnaswamy; Christ, David D.

CORPORATE SOURCE: Metabolism and Pharmacokinetics, Bristol-Myers Squibb Company, Wallingford, CT, USA

SOURCE: Drug Metabolism and Disposition (2004), 32(12), 1359-1369
CODEN: DMDSAI; ISSN: 0090-9556

PUBLISHER: American Society for Pharmacology and Experimental Therapeutics

DOCUMENT TYPE: Journal

LANGUAGE: English

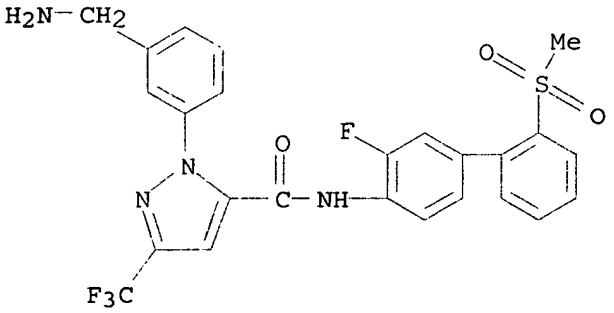
AB The chimpanzee (CHP) was evaluated as a pharmacokinetic model for humans (HUMs) using propranolol, verapamil, theophylline, and 12 proprietary compds. Species differences were observed in the systemic clearance of theophylline (.apprx.5-fold higher in CHPs), a low clearance compound, and the bioavailability of propranolol and verapamil (lower in CHPs), both high clearance compds. The systemic clearance of propranolol (.apprx.1.53 l/h/kg) suggested that the hepatic blood flow in CHPs is comparable to that in humans. No substantial differences were observed in the in vitro protein binding. A preliminary attempt was made to characterize cytochrome P 450 activities in CHP and HUM liver microsomes. Testosterone 6β-hydroxylation and tolbutamide methylhydroxylation activities were comparable in CHP and HUM liver microsomes. In contrast, dextromethorphan O-demethylation and phenacetin O-deethylation activities were .apprx.10-fold higher (per mg protein) in CHP liver microsomes. Intrinsic clearance ests. in CHP liver microsomes were higher for propranolol

(.apprx.10-fold) and theophylline (.apprx.5-fold) and similar for verapamil. Of the 12 proprietary compds., 3 had oral clearances that differed in the two species by more than 3-fold, an acceptable range for biol. variability. Most of the observed differences are consistent with species differences in P 450 enzyme activity. Oral clearances of proprietary compds. in HUMs were significantly correlated to those from CHPs (r = 0.68; p = 0.015), but not to ests. from rat, dog, and monkey. In summary, the chimpanzee serves as a valuable surrogate model for human pharmacokinetics, especially when species differences in P 450 enzyme activity are considered.

IT **292135-59-2**, DPC 423
RL: PKT (Pharmacokinetics); BIOL (Biological study)
(chimpanzee (Pan troglodytes) as a surrogate model for human pharmacokinetic studies in relation to species differences in P 450 enzyme activity)

RN 292135-59-2 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:950836 CAPLUS
DOCUMENT NUMBER: 140:16722
TITLE: Preparation of 1,1-disubstituted cycloalkyl derivatives as factor Xa inhibitors for treating a thromboembolic disorder
INVENTOR(S): Qiao, Jennifer X.; Pinto, Donald J.; Orwat, Michael J.; Han, Wei; Friedrich, Sarah R.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 686 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003099276	A1	20031204	WO 2003-US13893	20030505

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

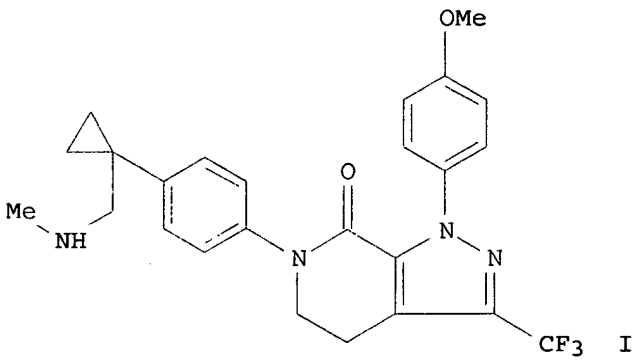
AU 2003273179	A1	20031212	AU 2003-273179	20030505
US 2004254158	A1	20041216	US 2003-430024	20030505
EP 1505966	A1	20050216	EP 2003-755341	20030505

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.:	US 2002-379357P	P	20020510
	US 2002-415367P	P	20021002
	WO 2003-US13893	W	20030505

OTHER SOURCE(S): MARPAT 140:16722

GI



I

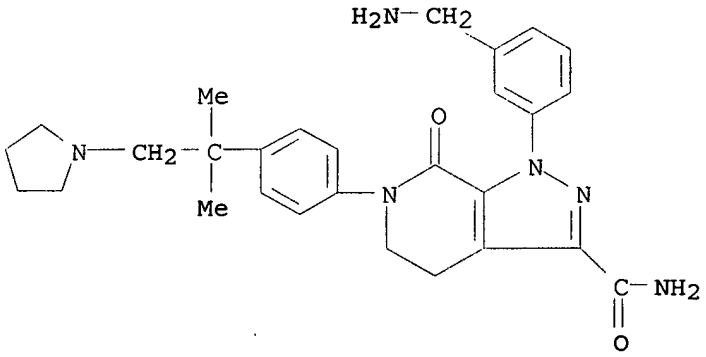
AB The present application describes 1,1-disubstituted cycloalkyl compds. and derivs. thereof (P4-P-M-M4; variables defined below; most of the examples contain 1,4,5,6-tetrahydro-7H-pyrazolo[3,4-c]pyridin-7-one, e.g. the trifluoroacetate of I), or pharmaceutically acceptable salt forms thereof, which are useful as inhibitors of factor Xa for treatment of a thromboembolic disorder. Although the methods of preparation are not claimed, .apprx.240 example prepns. are included. A number of I exhibit Ki's of <10 μM towards factor Xa; also some I are direct acting inhibitors (Ki < 10 μM) of the serine protease thrombin as indicated by their ability to inhibit the cleavage of small mol. substrates by thrombin in a purified system; the specific compds. are not stated. For I: M is a 3-10 membered carbocycle or a 4-10 membered heterocycle, consisting of: C atoms and 1-3 heteroatoms = O, S(O)p, N, and NZ2; ring M is substituted with 0-3 R1a and 0-2 carbonyl groups, and there are 0-3 ring double bonds; P is fused onto ring M and is a 5, 6, or 7 membered carbocycle or a 5, 6, or 7 membered heterocycle, consisting of: C atoms and 1-3 heteroatoms = O, S(O)p, and N; ring P is substituted with 0-3 R1a and 0-2 carbonyl groups, and there are 0-3 ring double bonds; alternatively, ring P is absent and P4 is directly attached to ring M, provided that when ring P is absent, P4 and M4 are attached to the 1,2, 1,3, or 1,4 positions of ring M. One of P4 and M4 is -Z-A-B and the other -G1-G, provided that P4 and M4 are attached to different rings when ring P is present; G is consists of 2 fused rings D

and E (ring D, including the two atoms of Ring E to which it is attached, is a 5-6 membered ring consisting of carbon atoms and 0-2 heteroatoms selected from the group consisting of N, O, and S(O)p; E is selected from (un)substituted Ph, pyridyl, pyrimidyl, pyrazinyl, and pyridazinyl; alternatively, ring D is absent and ring E is selected from (un)substituted Ph, pyridyl, pyrimidyl, pyrazinyl, pyridazinyl, pyrrolyl, pyrazolyl, imidazolyl, isoxazolyl, oxazolyl, triazolyl, thienyl, and thiazolyl); G1 is absent or = (CR3R3a)1-5, etc. A = (un)substituted C3-10 carbocycle and 5-12 membered heterocycle consisting of: C atoms and 1-4 heteroatoms N, O, and S(O)p; B is Y-R4a or X-Y-R4a, provided that Z and B are attached to different atoms on A and A and R4a or X and R4a are attached to the same atom on Y; Z = a bond, -(CR3R3e)1-4-, etc. Addnl. details including provisos are given in the claims.

IT **630386-81-1P 630386-82-2P 630386-94-6P**
630386-95-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of 1,1-disubstituted cycloalkyl derivs. as factor Xa inhibitors for treating thromboembolic disorder)

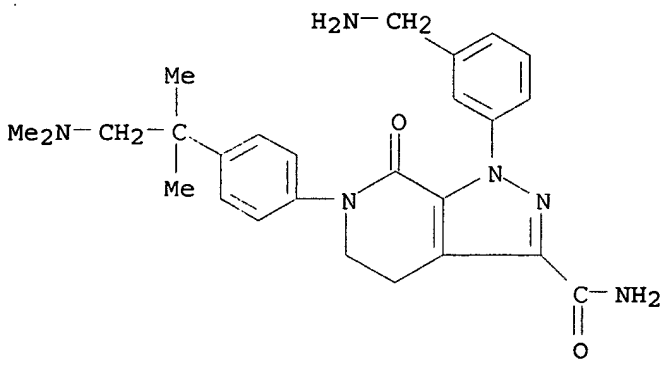
RN 630386-81-1 CAPLUS

CN 1H-Pyrazolo[3,4-c]pyridine-3-carboxamide, 1-[3-(aminomethyl)phenyl]-6-[4-[1,1-dimethyl-2-(1-pyrrolidinyl)ethyl]phenyl]-4,5,6,7-tetrahydro-7-oxo- (9CI) (CA INDEX NAME)

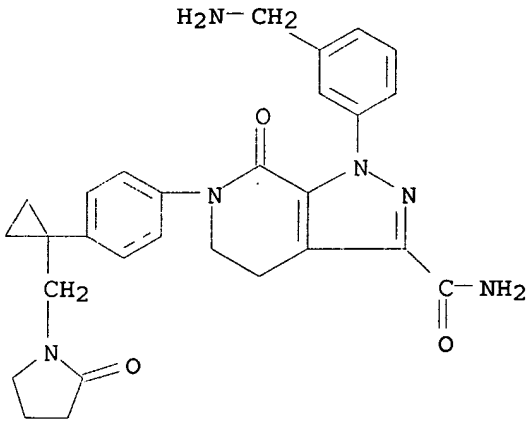


RN 630386-82-2 CAPLUS

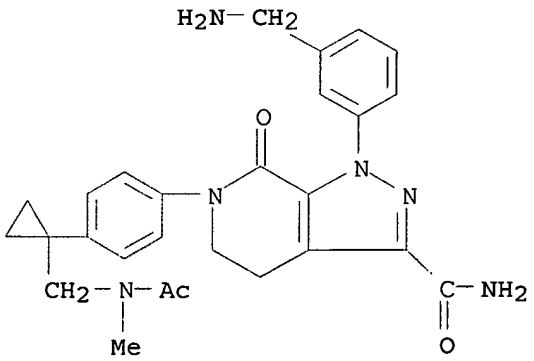
CN 1H-Pyrazolo[3,4-c]pyridine-3-carboxamide, 1-[3-(aminomethyl)phenyl]-6-[4-[2-(dimethylamino)-1,1-dimethylethyl]phenyl]-4,5,6,7-tetrahydro-7-oxo- (9CI) (CA INDEX NAME)



RN 630386-94-6 CAPLUS
CN 1H-Pyrazolo[3,4-c]pyridine-3-carboxamide, 1-[3-(aminomethyl)phenyl]-4,5,6,7-tetrahydro-7-oxo-6-[4-[1-[(2-oxo-1-pyrrolidinyl)methyl]cyclopropyl]phenyl]- (9CI) (CA INDEX NAME)



RN 630386-95-7 CAPLUS
CN 1H-Pyrazolo[3,4-c]pyridine-3-carboxamide, 6-[4-[1-[(acetylmethylamino)methyl]cyclopropyl]phenyl]-1-[3-(aminomethyl)phenyl]-4,5,6,7-tetrahydro-7-oxo- (9CI) (CA INDEX NAME)

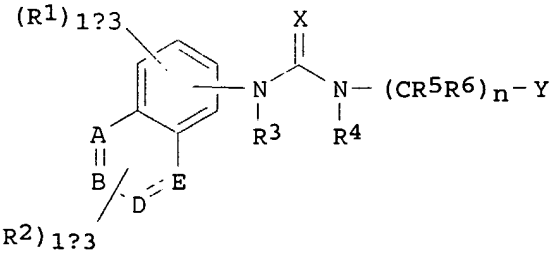


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:777762 CAPLUS
DOCUMENT NUMBER: 139:292162
TITLE: Heteroaromatic ureas as vanilloid receptor (VR1) modulators, in particular antagonists, for treating pain and/or inflammation
INVENTOR(S): Brown, Rebecca Elizabeth; Doughty, Victoria Alexandra; Hollingworth, Gregory John; Jones, A. Brian; Lindon, Matthew John; Moyes, Christopher Richard; Rogers, Lauren
PATENT ASSIGNEE(S): Merck Sharp & Dohme Limited, UK
SOURCE: PCT Int. Appl., 110 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003080578	A1	20031002	WO 2003-GB1302	20030321
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2479150	AA	20031002	CA 2003-2479150	20030321
AU 2003214442	A1	20031008	AU 2003-214442	20030321
EP 1490340	A1	20041229	EP 2003-710014	20030321
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005107388	A1	20050519	US 2003-505358	20030321
JP 2005526798	T2	20050908	JP 2003-578333	20030321
PRIORITY APPLN. INFO.:			GB 2002-6876 A	20020322
			WO 2003-GB1302 W	20030321

OTHER SOURCE(S): MARPAT 139:292162
GI



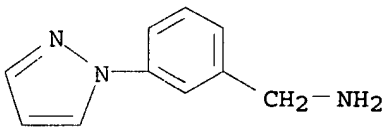
I

AB Title compds. I [wherein A, B, D, E are each C or N with the proviso that one or more are N; R1, R2 = independently H, halo, alk(enyl/ynyl), haloalkyl, hydroxyalkyl, cycloalkyl, cycloalkylalkyl, NH2 and derivs., CO2H and derivs., (un)substituted alkyl, alkoxy; R3, R4 = independently H, alk(en/yn)yl; R5, R6 = at each occurrence, independently H, alk(enyl/ynyl), alkoxy, acyloxy, carboxy and derivs., CONH2 and derivs., sulfonyl(alkyl/amino), aryl, hetero(aryl/cyclyl), (un)substituted alkyl; or CR5R6 = 3-6 carbocyclic membered ring; R7, R8 = at each occurrence, independently H, alk(en/yn)yl, cycloalkyl, fluoroalkyl; or NR7R8 = (un)substituted 4-7 heteroaliph. membered ring; X = O, S or =NCN; Y = aryl, heteroaryl, carbocyclyl, fused carbocyclyl group; n = 0, 1, 2, 3; and their pharmaceutically acceptable salts, N-oxides, and prodrugs] were prepared as vanilloid receptor (VR1) modulators, in particular antagonists, for treating conditions or diseases in which pain and/or inflammation predominates. For example, 1-isoquinolin-5-yl-3-(3-phenylpropyl)urea was prepared by reacting isoquinoline-5-carboxylic acid with diphenylphosphoryl azide in toluene at reflux for 1 h through a Curtius rearrangement, followed by addition of 3-phenylpropylamine and reflux for 18 h. I bound to the VR1 receptor with an IC50 < 1 μM, and in the majority of cases, < 200 nM. I are predominantly VR1 antagonists with a few of them VR1 partial antagonists and VR1 partial agonists. Thus, I and their pharmaceutical compns. are useful for treating pain and/or inflammation.

IT **608515-39-5P**, 3-(1H-Pyrazol-1-yl)benzylamine hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of heteroarom. ureas as vanilloid receptor modulators for treating pain and inflammation)

RN 608515-39-5 CAPLUS

CN Benzenemethanamine, 3-(1H-pyrazol-1-yl)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:261670 CAPLUS
DOCUMENT NUMBER: 138:287666
TITLE: Preparation of heteroaryllactams as Factor Xa inhibitors
INVENTOR(S): Pinto, Donald; Quan, Mimi; Orwat, Michael; Li, Yun-Long; Han, Wei; Qiao, Jennifer; Lam, Patrick; Koch, Stephanie
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 441 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003026652	A1	20030403	WO 2002-US29491	20020917
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2461202	AA	20030403	CA 2002-2461202	20020917
US 2003191115	A1	20031009	US 2002-245122	20020917
US 6967208	B2	20051122		
EP 1427415	A1	20040616	EP 2002-775843	20020917
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002012726	A	20040803	BR 2002-12726	20020917
CN 1578660	A	20050209	CN 2002-821537	20020917
JP 2005507889	T2	20050324	JP 2003-530289	20020917
ZA 2004002184	A	20050503	ZA 2004-2184	20040318
NO 2004001163	A	20040503	NO 2004-1163	20040319
US 2004220174	A1	20041104	US 2004-850587	20040520
US 6989391	B2	20060124		
US 2005124602	A1	20050609	US 2004-970781	20041021
US 7005435	B2	20060228		
US 2005171085	A1	20050804	US 2004-970807	20041021
US 6995172	B2	20060207		
US 2005261287	A1	20051124	US 2005-154972	20050616
US 2005267097	A1	20051201	US 2005-198801	20050805

PRIORITY APPLN. INFO.:	US 2001-324165P	P	20010921
	US 2002-402317P	P	20020809
	US 2002-245122	A3	20020917
	WO 2002-US29491	W	20020917
	US 2004-850587	A3	20040520
	US 2004-970807	A1	20041021

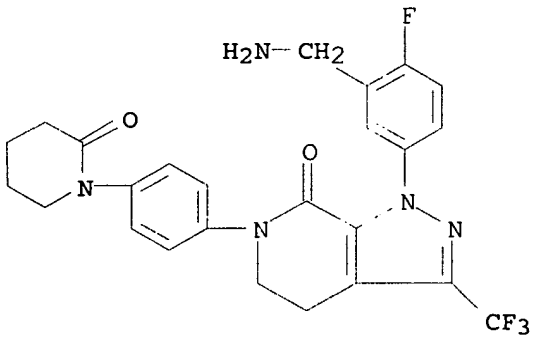
OTHER SOURCE(S): MARPAT 138:287666

AB P4PMM4 [M = 3-10 membered (substituted) (unsatd.) carbocyclyl, 4-10 membered heeterocyclyl; P = null, 5-7 membered (substituted) (unsatd.) carbocyclyl, heterocyclyl fused to ring M; 1 of P4, M4 = ZAB, the other = G1G; G = (benzo-, pyrido-, pyrimido-, pyrazino-, or pyridazino-fused) (substituted) (unsatd.) 5-6 membered (hetero)cyclyl; G1 = null, (CR3R3a)1-5, etc.; R3, R3a = H, Me, Et, Pr, Ph, PhCH2, etc.; Z = bond, (CR3R3e)1-4, etc.; R3e = H, SO2NHR3, SO2N(R3)2, COR3, (substituted) alkyl, alkenyl, alkynyl, etc.; A = (substituted) 3-10 membered carbocyclyl, 5-12 membered heterocyclyl; Z = XNQ; X = null, CO, SO, SO2, etc.; NQ = 4-8 membered mono- or bicyclic (substituted) (unsatd.) ring containing a CO or SO2 group adjacent to the N atom; with provisos], were prepared Thus, 6-(4-iodophenyl)-3-methoxy-1-(4-methoxyphenyl)-1,4,5,6-tetrahydro-7H-pyrazolo[3,4-c]pyridin-7-one (preparation given), δ-valerolactam, K2CO3, and CuI were refluxed in Me2SO to give 15% 3-methoxy-1-(4-methoxyphenyl)-6-[4-(2-oxo-1-piperidinyl)phenyl]-1,4,5,6-tetrahydro-7H-pyrazolo[3,4-c]pyridin-7-one. Several title compds. inhibited Factor Xa with IC50≤ 10 μM.

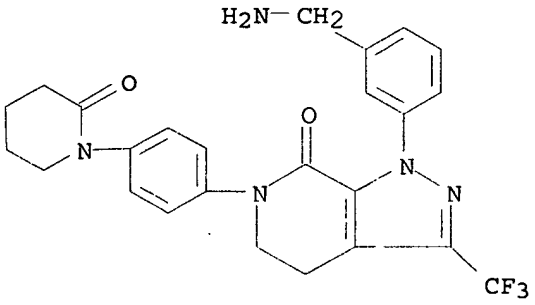
IT **503612-37-1P**, 1-(3-(Aminomethyl)-4-fluorophenyl)-6-[4-(2-oxo-1-

piperidinyl)phenyl]-3-(trifluoromethyl)-1,4,5,6-tetrahydro-7H-pyrazolo[3,4-c]pyridine-7-one **503612-59-7P**, 1-[3-(Aminomethyl)phenyl]-6-[4-(2-oxo-1-piperidinyl)phenyl]-3-(trifluoromethyl)-1,4,5,6-tetrahydro-7H-pyrazolo[3,4-c]pyridin-7-one **503613-00-1P**, 1-(3-Aminomethyl-4-fluorophenyl)-7-oxo-6-[4-(2-oxo-1-piperidinyl)phenyl]-4,5,6,7-tetrahydro-1H-pyrazolo[3,4-c]pyridine-3-carboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of heteroaryllactams as Factor Xa inhibitors)

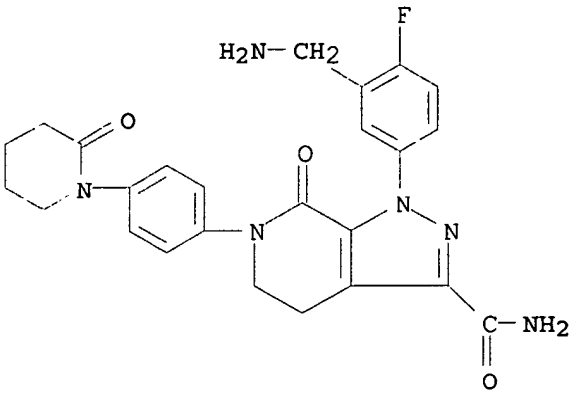
RN 503612-37-1 CAPLUS
CN 7H-Pyrazolo[3,4-c]pyridin-7-one, 1-[3-(aminomethyl)-4-fluorophenyl]-1,4,5,6-tetrahydro-6-[4-(2-oxo-1-piperidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 503612-59-7 CAPLUS
CN 7H-Pyrazolo[3,4-c]pyridin-7-one, 1-[3-(aminomethyl)phenyl]-1,4,5,6-tetrahydro-6-[4-(2-oxo-1-piperidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



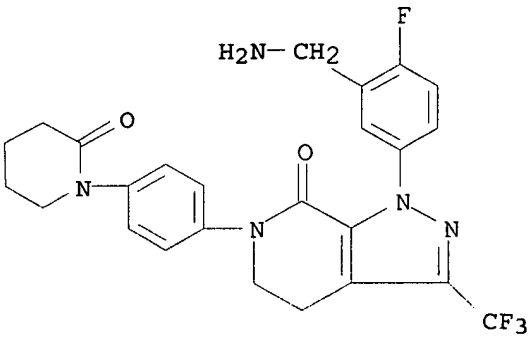
RN 503613-00-1 CAPLUS
CN 1H-Pyrazolo[3,4-c]pyridine-3-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-4,5,6,7-tetrahydro-7-oxo-6-[4-(2-oxo-1-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)



IT **503615-15-4P 503615-24-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heteroaryllactams as Factor Xa inhibitors)
RN 503615-15-4 CAPLUS
CN 7H-Pyrazolo[3,4-c]pyridin-7-one, 1-[3-(aminomethyl)-4-fluorophenyl]-1,4,5,6-tetrahydro-6-[4-(2-oxo-1-piperidinyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

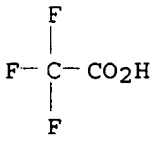
CM 1

CRN 503612-37-1
CMF C25 H23 F4 N5 O2



CM 2

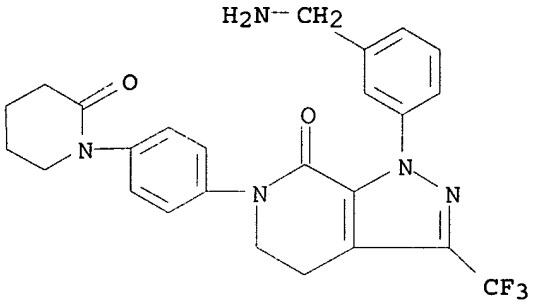
CRN 76-05-1
CMF C2 H F3 O2



RN 503615-24-5 CAPLUS
CN 7H-Pyrazolo[3,4-c]pyridin-7-one, 1-[3-(aminomethyl)phenyl]-1,4,5,6-tetrahydro-6-[4-(2-oxo-1-piperidinyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

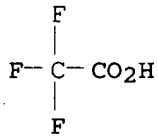
CM 1

CRN 503612-59-7
CMF C25 H24 F3 N5 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 15 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:844982 CAPLUS
DOCUMENT NUMBER: 140:59557
TITLE: Discovery of 1-(2-Aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl)]-4-yl]-1H-pyrazole-5-carboxamide (DPC602), a Potent, Selective, and Orally Bioavailable Factor Xa Inhibitor
AUTHOR(S): Pruitt, James R.; Pinto, Donald J. P.; Galemmo, Robert A., Jr.; Alexander, Richard S.; Rossi, Karen A.; Wells, Brian L.; Drummond, Spencer; Bostrom, Lori L.; Burdick, Debra; Bruckner, Robert; Chen, Haiying; Smallwood, Angela; Wong, Pancras C.; Wright, Matthew R.; Bai, Steven; Luettgen, Joseph M.; Knabb, Robert M.; Lam, Patrick Y. S.; Wexler, Ruth R.
CORPORATE SOURCE: Pharmaceutical Research Institute, Bristol-Myers Squibb Company, Pennington, NJ, 08534, USA
SOURCE: Journal of Medicinal Chemistry (2003), 46(25), 5298-5315

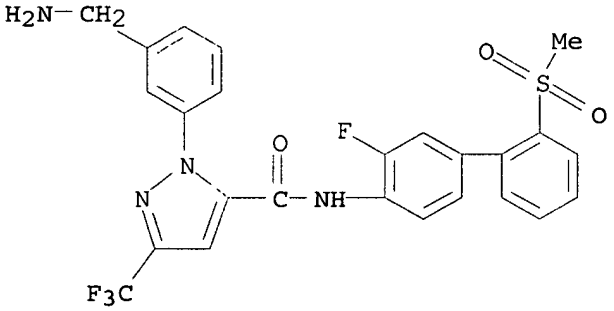
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:59557

AB Factor Xa, a serine protease, is at the critical juncture between the intrinsic and extrinsic pathways of the coagulation cascade. Inhibition of factor Xa has the potential to provide effective treatment for both venous and arterial thrombosis. The authors recently described a series of meta-substituted phenylpyrazoles that are highly potent, selective, and orally bioavailable factor Xa inhibitors. In this paper, the authors report their efforts to further optimize the selectivity profile of the factor Xa inhibitors with a series of ortho- and/or para-substituted phenylpyrazole derivs. The most potent compds. display sub-nanomolar inhibition consts. for factor Xa and show greater than 1000-fold selectivity against other serine proteases. These compds. are also effective in a rabbit model of arteriovenous shunt thrombosis. Optimization of this series led to the preclin. development of DPC602, a 2-(aminomethyl)phenylpyrazole analog, as a highly potent, selective, and orally bioavailable factor Xa inhibitor.

IT **209957-47-1DP**, factor Xa complex
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure of)

RN 209957-47-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



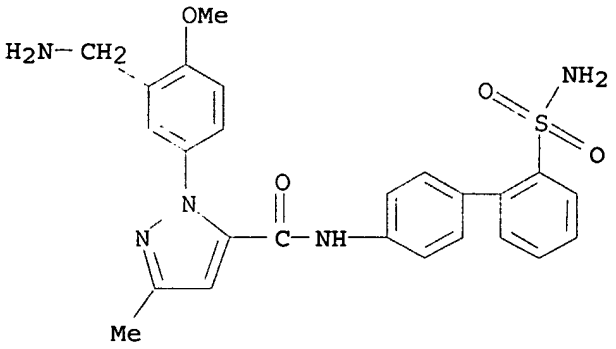
IT **637318-44-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of 1-(2-aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl)]-4-yl]-1H-pyrazole-5-carboxamide and related compds. as orally bioavailable factor Xa inhibitors)

RN 637318-44-6 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

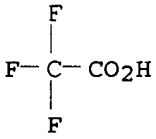
CM 1

CRN 637318-43-5
CMF C25 H25 N5 O4 S

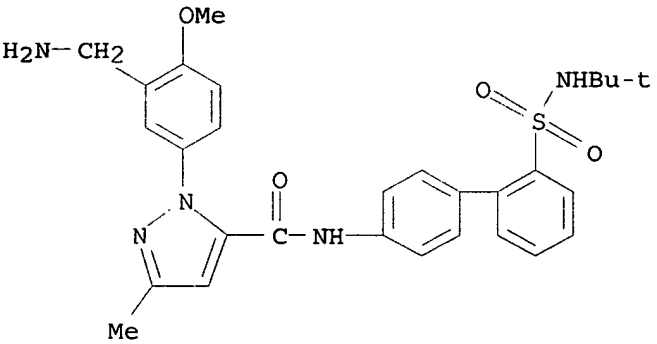


CM 2

CRN 76-05-1
CMF C2 H F3 O2



IT **637318-46-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-(2-aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl)]-4-yl]-1H-pyrazole-5-carboxamide and related compds. as orally bioavailable factor Xa inhibitors)
RN 637318-46-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-methoxyphenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



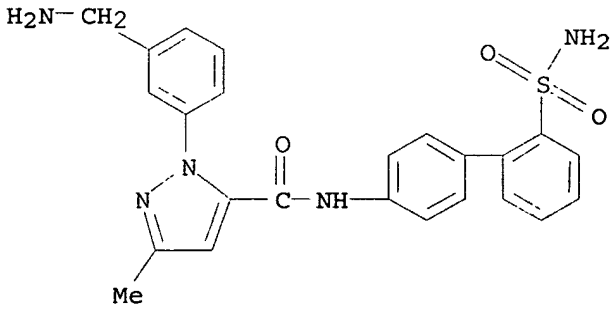
REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 16 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:784065 CAPLUS

DOCUMENT NUMBER: 140:12453
TITLE: Structure-based design of novel guanidine/benzamidine mimics: potent and orally bioavailable factor Xa inhibitors as novel anticoagulants
AUTHOR(S): Lam, Patrick Y. S.; Clark, Charles G.; Li, Renhua; Pinto, Donald J. P.; Orwat, Michael J.; Galemmo, Robert A.; Fevig, John M.; Teleha, Christopher A.; Alexander, Richard S.; Smallwood, Angela M.; Rossi, Karen A.; Wright, Matthew R.; Bai, Stephen A.; He, Kan; Luettgen, Joseph M.; Wong, Pancras C.; Knabb, Robert M.; Wexler, Ruth R.
CORPORATE SOURCE: Bristol-Myers Squibb Company, Princeton, NJ, 08542-5400, USA
SOURCE: Journal of Medicinal Chemistry (2003), 46(21), 4405-4418
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:12453

AB As part of an ongoing effort to prepare orally active factor Xa inhibitors using structure-based drug design techniques and mol. recognition principles, a systematic study has been performed on the pharmacokinetic profile resulting from replacing the benzamidine in the P1 position with less basic benzamidine mimics or neutral residues. It is demonstrated that lowering the pKa of the P1 ligand resulted in compds. (3-benzylamine, 15a; 1-aminoisoquinoline, 24a; 3-aminobenzisoxazole, 23a; 3-phenylcarboxamide, 22b; and 4-methoxyphenyl, 22a) with improved pharmacokinetic features mainly as a result of decreased clearance, increased volume of distribution, and enhanced oral absorption. This work resulted in a series of potent and orally bioavailable factor Xa inhibitors that ultimately led to the discovery of SQ311, 24a. SQ311, which utilizes a 1-aminoisoquinoline as the P1 ligand, inhibits factor Xa with a Ki of 0.33 nM and demonstrates both good in vivo antithrombotic efficacy and oral bioavailability.

IT **209955-58-8**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(guanidine/benzamidine mimics as potent and orally bioavailable factor Xa inhibitors and anticoagulants)
RN 209955-58-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)

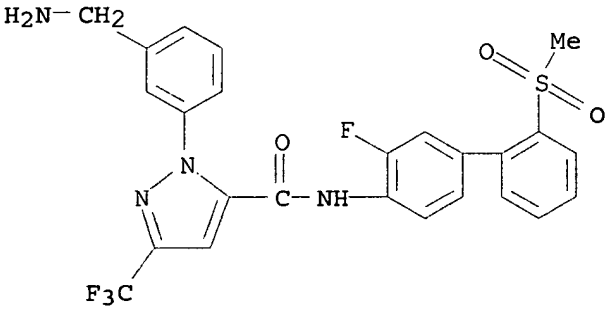


REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 17 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:363518 CAPLUS
DOCUMENT NUMBER: 140:16
TITLE: Factor Xa inhibitors: Today and beyond
AUTHOR(S): Walenga, Jeanine M.; Jeske, Walter P.; Hoppensteadt, Debra; Fareed, Jawed
CORPORATE SOURCE: Department of Pathology, Loyola University Medical Center, Maywood, IL, 60153, USA
SOURCE: Current Opinion in Investigational Drugs (Thomson Current Drugs) (2003), 4(3), 272-281
CODEN: COIDAZ; ISSN: 1472-4472
PUBLISHER: Thomson Current Drugs
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review. Serine proteases play an important role in thrombogenesis, the process that leads to blood clotting and conditions such as heart attack, stroke and other cardiovascular disorders. In the coagulation network, the activation of various serine proteases facilitates the formation of the serine protease Factor Xa, which plays a central role in the process of coagulation and platelet activation. Factor Xa is an essential component of the prothrombinase complex, from which thrombin is formed, which then directly leads to fibrin clot formation. Thus, the inhibition of Factor Xa and its generation is an important strategy in the development of new antithrombotic drugs.

IT **292135-59-2**, DPC-423
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(factor Xa inhibitors as antithrombotic drugs)
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 120 THERE ARE 120 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 18 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:85815 CAPLUS
DOCUMENT NUMBER: 138:395309
TITLE: Development and validation of a liquid

chromatography-mass spectrometric method for the determination of DPC 423, an antithrombotic agent, in rat and dog plasma

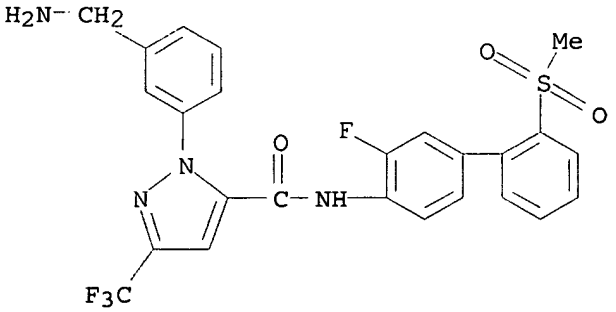
AUTHOR(S): Chi, Cecilia; Liang, Li; Padovani, Patty; Unger, Steve
CORPORATE SOURCE: Metabolism & Pharmacokinetics, PRI, Experimental Station, Bristol-Myers Squibb Company, Wilmington, DE, 19803-0353, USA

SOURCE: Journal of Chromatography, B: Analytical Technologies in the Biomedical and Life Sciences (2003), 783(1), 163-172
CODEN: JCBAAI; ISSN: 1570-0232
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A sensitive and selective LC-MS-MS method for the determination of DPC 423 (I), an antithrombotic agent, is described. This method used a solid-phase extraction from 0.1 mL plasma with an Isolute C2 cartridge. HPLC separation was carried out on a YMC ODS-AQ C18 column (50+2 mm) at a flow rate of 300 μL/min with an anal. time of 5 min. Compds. were eluted using a mobile phase of H2O/CH3CN/HCOOH:66:34:0.1 (volume/volume/volume), pH 4.0. A structural analog of I was used as the internal standard to account for variations in recovery and instrument response. Mass spectrometric detection was carried out with a PE Sciex API III+ triple quadrupole mass spectrometer equipped with a Turbo IonSpray source as the LC-MS interface. Good intraday and interday assay precision (<10% CV) and accuracy (<10% difference) were observed over a concentration range of 0.005-2.5 μM in plasma. The extraction recoveries were .apprx.90% and the method was found to be linear for the assay (r2>0.999). The method has been successfully applied to discovery and preclin. pharmacokinetic studies, including a dose range-finding study and toxicokinetic exposure studies in rat and dog.

IT **292135-59-2**, DPC 423
RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)
(development and validation of liquid chromatog.-mass spectrometric method for determination of DPC 423 in rat and dog plasma)

RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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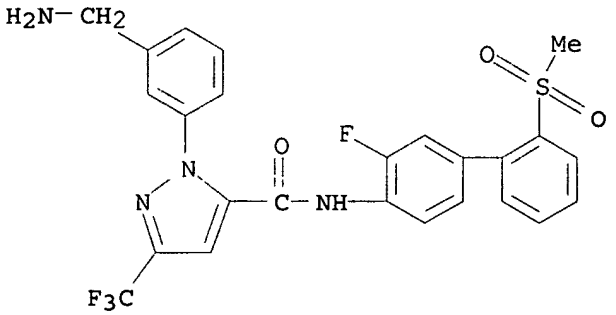
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 19 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:932561 CAPLUS
DOCUMENT NUMBER: 138:378909
TITLE: Nonpeptide factor Xa inhibitors III: effects of DPC423, an orally-active pyrazole antithrombotic agent, on arterial thrombosis in rabbits
AUTHOR(S): Wong, Pancras C.; Crain, Earl J.; Watson, Carol A.; Zaspel, Alverna M.; Wright, Matthew R.; Lam, Patrick Y.; Pinto, Donald J. P.; Wexler, Ruth R.; Knabb, Robert M.
CORPORATE SOURCE: Cardiovascular Biology, Bristol-Myers Squibb Company, Wilmington, DE, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (2002), 303(3), 993-1000
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB DPC423 [1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide] is a synthetic, competitive, and selective inhibitor of coagulation factor Xa (fXa) (Ki: 0.15 nM in humans, 0.3 nM in rabbit). The objective of this study was to compare effects of DPC423, enoxaparin (low-mol.-weight heparin), and argatroban (thrombin inhibitor) on arterial thrombosis and hemostasis in rabbit models of elec. induced carotid artery thrombosis and cuticle bleeding, resp. Compds. were infused i.v. continuously from 60 min before artery injury or cuticle transection to the end of experiment Carotid blood flow was used as a marker of antithrombotic effect. Antithrombotic ED50 values were 0.4 mg/kg/h for enoxaparin (n = 6), 0.13 mg/kg/h for argatroban (n = 6), and 0.6 mg/kg/h for DPC423 (n = 12). DPC423 at the maximum antithrombotic dose increased activated partial thromboplastin time and prothrombin time (n = 6) by 1.8 ± 0.07- and 1.8 ± 0.13-fold, resp., without changes in thrombin time and ex vivo thrombin activity. The antithrombotic effect of DPC423 was significantly correlated with its ex vivo anti-fXa activity (r = 0.86). DPC423 at 1, 3, and 10 mg/kg p.o. increased carotid blood flow (percent control) at 45 min to 10 ± 4, 24 ± 6, and 74 ± 7, resp. (n = 6/group). Cuticle bleeding times (percent change over control) determined at the maximum antithrombotic dose were 88 ± 12 for argatroban, 69 ± 13 for heparin, 4 ± 3 for enoxaparin, 5 ± 4 for DPC423, and -3 ± 2 for the vehicle (n = 5-6/group), suggesting dissociation of antithrombotic and bleeding time effects for DPC423 and enoxaparin. The combination of aspirin and DPC423 at ineffective antithrombotic doses produced significant antithrombotic effect. Therefore, these results suggest that DPC423 is a clin. useful oral anticoagulant for the prevention of arterial thrombosis.

IT **292135-59-2**, DPC423
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(factor Xa inhibitors: orally-active pyrazole antithrombotic agent DPC423)

RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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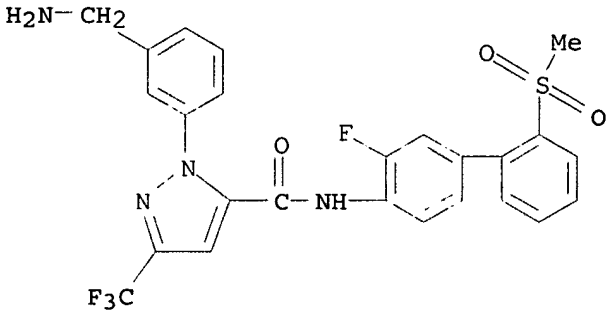
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 20 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:621918 CAPLUS
DOCUMENT NUMBER: 138:147036
TITLE: DPC-423 (Bristol-Myers squibb)
AUTHOR(S): Taglialatela, Maurizio
CORPORATE SOURCE: Section of Pharmacology, Department of Neuroscience, University of Naples "Federico II", Naples, 80131, Italy
SOURCE: Current Opinion in Investigational Drugs (PharmaPress Ltd.) (2002), 3(2), 252-254
CODEN: COIDAZ; ISSN: 1472-4472
PUBLISHER: PharmaPress Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. DPC-423 is a biphenylamine-containing amide which is under development by Bristol-Myers Squibb (formerly DuPont Pharmaceuticals) as a Factor Xa inhibitor for the potential treatment of thrombotic disorders. As of August 2000, DPC-423 was in phase I trials. DPC-423 was discovered as a result of SAR modifications of DuPont's SN-429, including replacement of the benzamidine moiety with a less basic benzylamine. Its 2-aminomethylphenyl analog DPC-602 is also under investigation for thrombotic disorders.
IT **292135-59-2**, DPC-423
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(DPC-423 a factor Xa inhibitor)
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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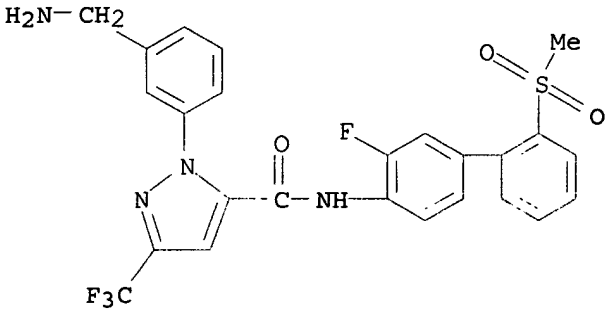
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 21 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:845163 CAPLUS
DOCUMENT NUMBER: 139:79
TITLE: Nonpeptide factor Xa inhibitors: DPC423, a highly potent and orally bioavailable pyrazole antithrombotic agent
AUTHOR(S): Wong, Pancras C.; Pinto, Donald J. P.; Knabb, Robert M.
CORPORATE SOURCE: Cardiovascular Biology, Bristol-Myers Squibb Company, Wilmington, DE, USA
SOURCE: Cardiovascular Drug Reviews (2002), 20(2), 137-152
CODEN: CDREEA; ISSN: 0897-5957
PUBLISHER: Neva Press
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. DPC 423 is a synthetic, orally bioavailable, competitive, and selective inhibitor of human coagulation factor Xa (Ki [nM]: factor Xa, 0.15; trypsin, 60; thrombin, 6000; plasma kallikrein, 61; activated protein C, 1800; factor IXa, 2200; factor VIIa, >15,000; chymotrypsin, >17,000; urokinase, >19,000; plasmin, >35,000; tissue plasminogen activator, >45,000; complement factor I, 44,000 [IC50]). In vitro, DPC 423 produced anticoagulant effects in human plasma in which it doubled prothrombin time, activated partial thromboplastin time, and Heptest clotting time at 3.1, 3.1, and 1.1 μM, resp. In dogs, DPC 423 had a good pharmacokinetic profile with an oral bioavailability of 57%, a plasma clearance of 0.24 L/kg/h, and a plasma half-life of 7.5 h. In rabbit and rat models of arteriovenous shunt thrombosis, DPC 423 was an effective antithrombotic agent with an IC50 of 150 and 470 nM, resp. The antithrombotic effect of DPC 423 is likely to be related to the inhibition of factor Xa but not to the inhibition of thrombin or due to direct inhibition of platelet aggregation. Therefore, based on potency, selectivity, efficacy, and oral bioavailability, DPC 423 was selected for clin. development as an oral anticoagulant for the potential treatment of thrombotic disorders. Preliminary human data suggest that DPC 423 is orally bioavailable in humans and has a long plasma half-life.
IT **292135-59-2**, DPC 423
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(DPC 423 as factor Xa inhibitor and highly potent and orally bioavailable antithrombotic agent)

RN 292135-59-2 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 22 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:881166 CAPLUS

DOCUMENT NUMBER: 136:144634

TITLE: P450-mediated metabolism of 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)- [1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole- 5-carboxamide (DPC 423) and its analogs to aldoximes. Characterization of glutathione conjugates of postulated intermediates derived from aldoximes

AUTHOR(S): Mutlib, Abdul E.; Chen, Shiang-Yuan; Espina, Robert J.; Shockcor, John; Prakash, Shimoga R.; Gan, Liang-Shang

CORPORATE SOURCE: Drug Metabolism and Pharmacokinetics Section, DuPont Pharmaceuticals Company, Stine-Haskell Research Center, Newark, DE, 19714, USA

SOURCE: Chemical Research in Toxicology (2002), 15(1), 63-75
CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

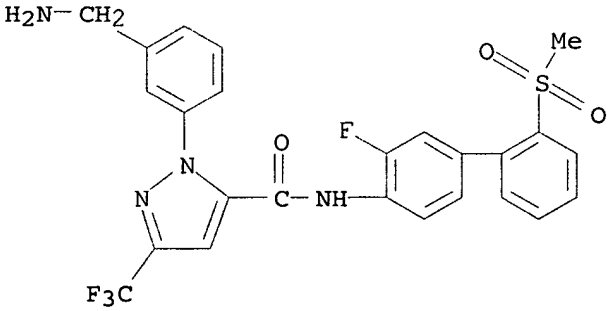
AB The in vivo and in vitro disposition of DPC 423, a highly potent, selective, and orally bioavailable inhibitor of blood coagulation factor Xa, has recently been described. Several metabolites, some of which were considered potentially reactive, were identified in rats. A novel GSH adduct, the structure of which was not determined conclusively, was isolated from bile of rats dosed with DPC 423. Herein, we describe the complete structural elucidation of this unique GSH conjugate employing LC/MS and high-field NMR. Similar GSH adducts of DPC 602, [13CD2]DPC 602, and SX 737, all structural analogs of DPC 423, were isolated, characterized spectroscopically, and shown to have identical mass fragmentation pathways. The structures of these conjugates were initially suspected to be either an amide with N-S bond or a nitrogen-oxygen juxtaposed amide

with a C-S bond. Studies conducted with [13CD2]DPC 602 indicated an aldoxime structure. The concluding evidence came from HMBC NMR spectrum of the conjugate, which showed strong correlation of the cysteine methylene protons with the imino carbon. Further spectroscopic studies with chemical prepared GSH adduct from benzaldehyde oxime confirmed this pattern of correlation. In vivo and in vitro studies with the synthetic oxime intermediate from DPC 423 showed an adduct identical to the one isolated from the bile of rats dosed with DPC 423. This supported the intermediacy of an aldoxime as a precursor to the GSH adducts. It is postulated that the benzylamine moiety of DPC 423 (and its analogs) is oxidized to a hydroxylamine, which is subsequently converted to a nitroso intermediate. Subsequent rearrangement of the nitroso leads to an aldoxime which in turn is metabolized by P 450 to a reactive intermediate. The formation of oxime from DPC 423 (and its analogs) was found to be mediated by rat CYP 3A1/2, which were also responsible for converting the oxime to the GSH trappable reactive intermediate. It is postulated that the aldoxime produces a radical or a nitrile oxide intermediate that reacts with GSH and hence produces this unusual GSH adduct. On the basis of synthetic analogy, it is more likely that the nitrile oxide resulting from two-electron oxidation of the aldoxime is the reactive intermediate. Intramol. kinetic isotope effects were studied with [13CD2]DPC 602 to assess the importance of the metabolic cleavage of the aminomethyl carbon-hydrogen bond in forming this GSH adduct. The lack of isotope effect in forming the aldoxime from [13CD2]DPC 602 suggests its formation does not occur through the imine intermediate. Instead the data supports the postulated mechanism of hydroxylamine and nitroso intermediates as precursors to the aldoxime. However, the formation of the GSH adduct from [13CD2]DPC 602 did show a significant intramol. kinetic isotope effect (kH/kD = 2.3) since a carbon-deuterium bond had to be broken on the aldoxime prior to the formation of the adduct. A stable nitrile oxide derived from DPC 602 was postulated as the reactive intermediate responsible for forming this unique GSH adduct.

IT **292135-59-2P**, DPC 423
RL: PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(P 450-mediated metabolism of blood coagulation factor Xa inhibitor DPC 423 and its analogs to aldoximes: characterization of glutathione conjugates)

RN 292135-59-2 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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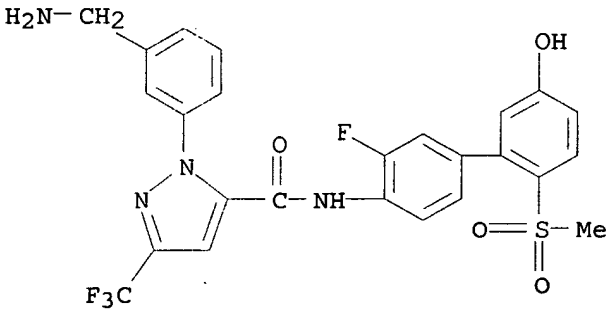
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 23 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:881167 CAPLUS
DOCUMENT NUMBER: 136:160835
TITLE: Disposition of 1-[3-(Aminomethyl)phenyl]-N-[3-fluoro-2'- (methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- 1H-pyrazole-5-carboxamide (DPC 423) by Novel Metabolic Pathways. Characterization of Unusual Metabolites by Liquid Chromatography/Mass Spectrometry and NMR
AUTHOR(S): Mutlib, Abdul. E.; Shockcor, John; Chen, Shiang-Yuan; Espina, Robert J.; Pinto, Donald J.; Orwat, Michael J.; Prakash, Shimoga R.; Gan, Liang-Shang
CORPORATE SOURCE: Drug Metabolism and Pharmacokinetics Section, DuPont Pharmaceuticals Company Stine-Haskell Research Center, Newark, DE, 19714, USA
SOURCE: Chemical Research in Toxicology (2002), 15(1), 48-62
CODEN: CRTOEC; ISSN: 0893-228X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The in vitro and in vivo disposition of DPC 423 was investigated in mice, rats, dogs and humans and the metabolites characterized by LC/MS, LC/NMR and high field-NMR. The rodents produced several metabolites that included an aldehyde (M1), a carboxylic acid (M2), a benzyl alc. (M3), glutamate conjugates (M4 and M5), an acyl glucuronide (M6) and its isomers; a carbamyl glucuronide (M7); a phenol (M8) and its glucuronide conjugate (M9), two glutathione adducts (M10 and M11), a sulfamate conjugate (M12), isomers of an oxime metabolite (M13), and an amide (M14). Humans and dogs produced less complex metabolite profiles than rats. While unchanged DPC 423 was the major component in plasma and urine samples, differences in the metabolic disposition of this compound among species were noted. M1 is believed to be rapidly oxidized to the carboxylic acid (M2), which forms the potentially reactive acyl glucuronide (M6). The formation of novel glutamate conjugates (M4 and M5) and their role in depleting endogenous glutathione have been described previously. The carbamyl glucuronide M7, found as the major metabolite in rats and in other species, was considered nonreactive and was easily hydrolyzed to the parent compound in the presence of β-glucuronidase. The identification of GSH adducts M10 and M11 led us to postulate the existence of at least two reactive intermediates responsible for their formation, an epoxide and possibly a nitrile oxide, resp. Although the formation of GSH adducts such as M10 from epoxides has been described before, there are no reports to date describing the existence of a GSH adduct (M11) of an oxime. The formation of a sulfamate conjugate (M12) formed by direct coupling of sulfate to the nitrogen of benzylamine is described. A mechanism is proposed for the formation of the oxime (M13) that involves sequential oxidation of the benzylamine to the corresponding hydroxylamine and nitroso intermediate. The rearrangement of the nitroso intermediate is believed to produce the oxime (M13). In vitro studies suggested that both the oxime (M13) and the aldehyde (M1) were precursors to the carboxylic acid (M2). This is the first demonstration of carboxylic acid formation via an oxime intermediate produced from an amine. The stability of DPC423 in plasma obtained from several species was studied. Significant species differences in the plasma stability of DPC 423 were observed The formation of the aldehyde metabolite (M1) was found to be catalyzed by a semicarbazide-sensitive monoamine oxidase

(SSAO) found in plasma of rabbits, dogs, and rhesus monkeys. Rat, chimpanzee, and human plasma did not form M1.

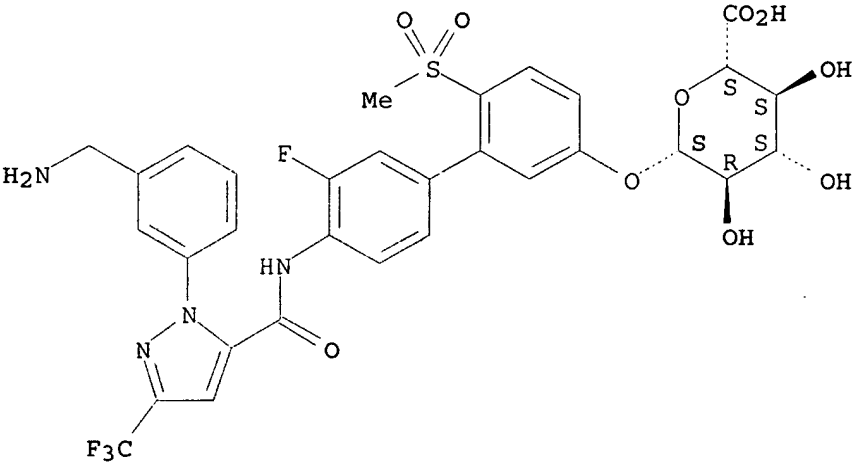
IT **397249-94-4 397249-95-5 397249-96-6**
RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)
(disposition of DPC 423 by novel metabolic pathways and characterization of unusual metabolites by liquid chromatog./mass spectrometry and NMR)

RN 397249-94-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-5'-hydroxy-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)



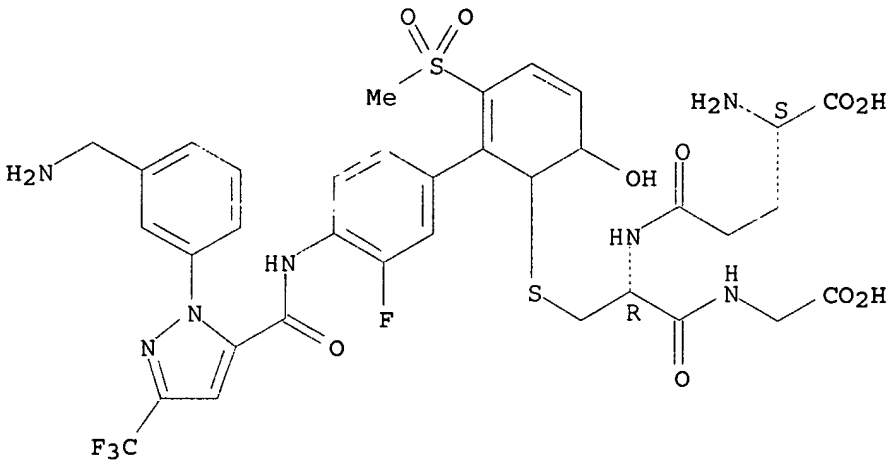
RN 397249-95-5 CAPLUS
CN β-D-Glucopyranosiduronic acid, 4'-[[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-3'-fluoro-6-(methylsulfonyl)[1,1'-biphenyl]-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

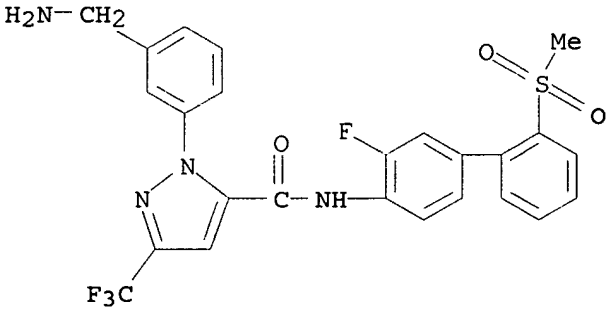


RN 397249-96-6 CAPLUS
CN Glycine, L-γ-glutamyl-S-[2-[4-[[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-3-fluorophenyl]-6-hydroxy-3-(methylsulfonyl)-2,4-cyclohexadien-1-yl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **292135-59-2**, DPC 423
RL: PKT (Pharmacokinetics); BIOL (Biological study)
(disposition of DPC 423 by novel metabolic pathways and characterization of unusual metabolites by liquid chromatog./mass spectrometry and NMR)
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

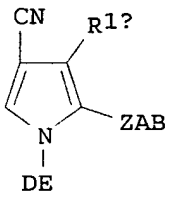
L7 ANSWER 24 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:338499 CAPLUS
DOCUMENT NUMBER: 134:348280
TITLE: Cyano compounds as factor Xa inhibitors
INVENTOR(S): Pinto, Donald J. P.
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

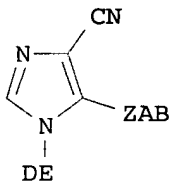
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032628	A1	20010510	WO 2000-US30209	20001102
W: US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
US 6407256	B1	20020618	US 2000-686382	20001011
EP 1226123	A1	20020731	EP 2000-976822	20001102
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				

PRIORITY APPLN. INFO.: US 1999-163268P P 19991103
WO 2000-US30209 W 20001102

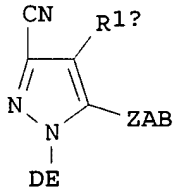
OTHER SOURCE(S): MARPAT 134:348280
GI



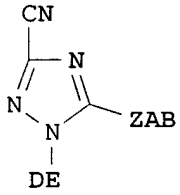
Ia



Ib



Ic



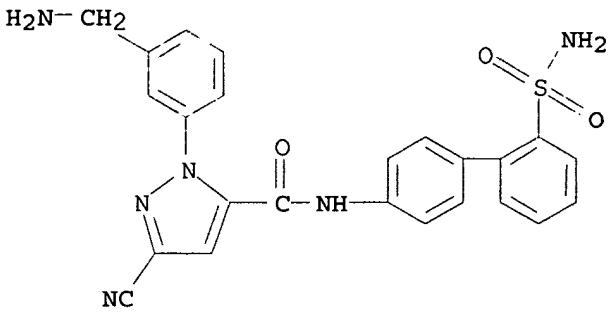
Id

AB The present application describes inhibitors of factor Xa which are cyano-pyrazole, cyano-triazole, cyano-imidazole, and cyano-pyrrole compds. of Formulas Ia, Ib, Ic, and Id: or pharmaceutically acceptable salt forms thereof. Markush structures and exemplary compds. of the invention are given (no data).

IT **338946-69-3 338946-70-6 338946-71-7**
338946-72-8 338946-73-9 338946-74-0
338946-75-1 338946-76-2 338946-77-3
338946-78-4 338946-79-5 338946-80-8
338946-81-9 338946-82-0 338946-83-1
338946-84-2 338946-85-3 338946-86-4
338946-87-5 338946-88-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cyano compds. as factor Xa inhibitors)

RN 338946-69-3 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-cyano- (9CI) (CA INDEX NAME)



RN 338946-70-6 CAPLUS
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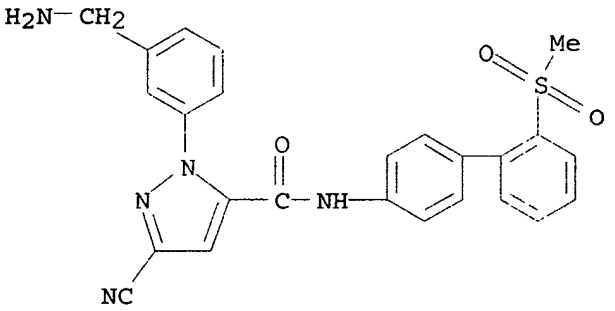
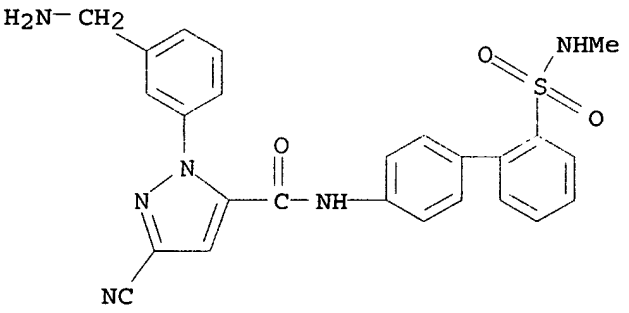
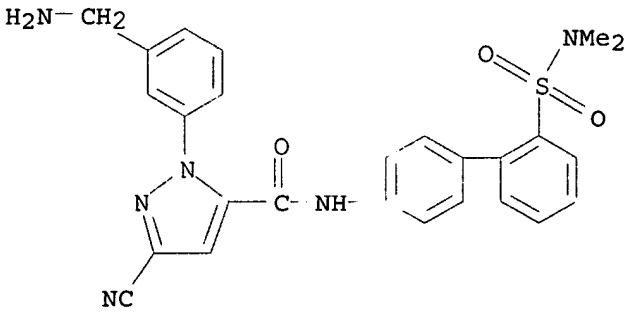


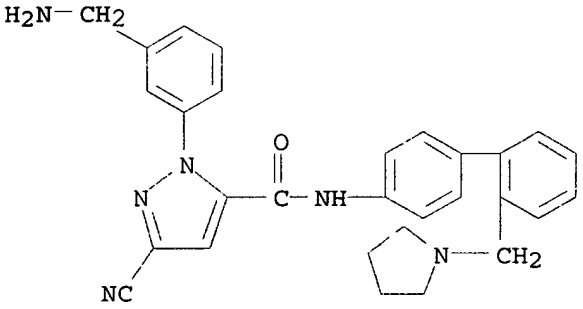
RN 338946-71-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2'-[(methylamino)sulfonyl][1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



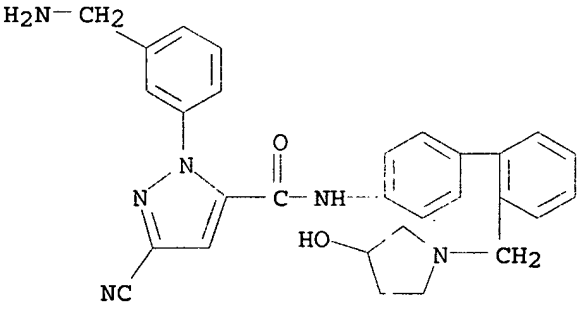
RN 338946-72-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2'-[(dimethylamino)sulfonyl][1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



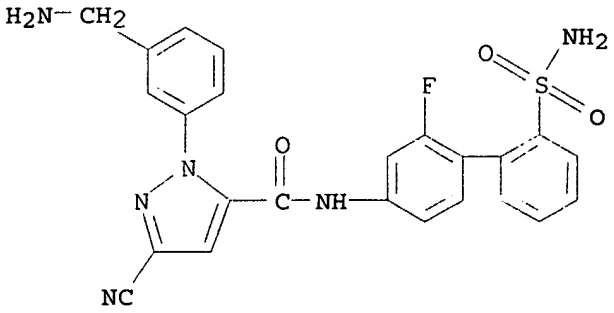
RN 338946-73-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2'-(1-pyrrolidinylmethyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



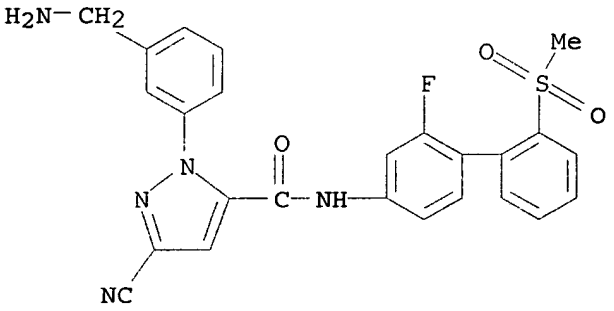
RN 338946-74-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2'-[(3-hydroxy-1-pyrrolidinyl)methyl][1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



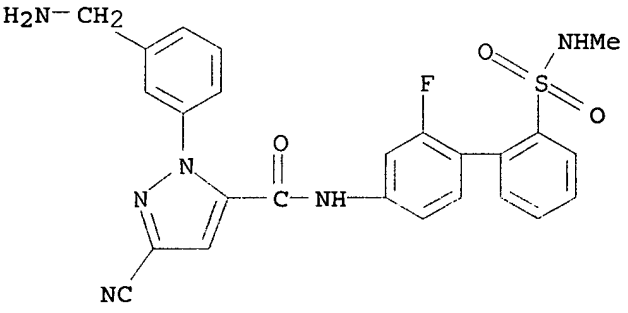
RN 338946-75-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-2-fluoro[1,1'-biphenyl]-4-yl]-3-cyano- (9CI) (CA INDEX NAME)



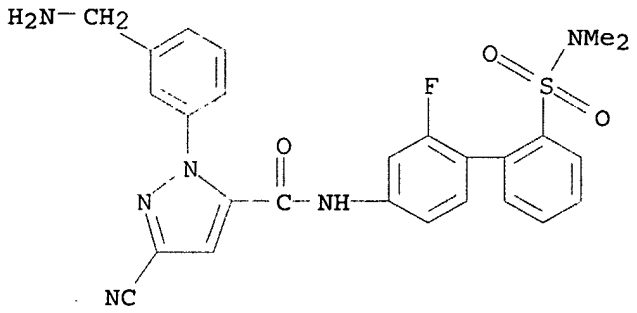
RN 338946-76-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



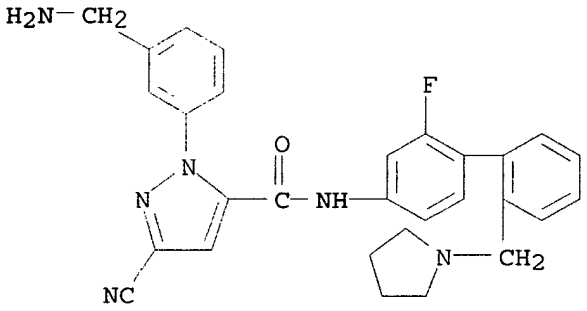
RN 338946-77-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2-fluoro-2'-[(methylamino)sulfonyl][1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



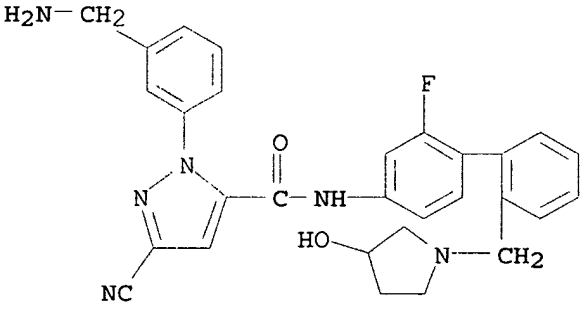
RN 338946-78-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2'-[(dimethylamino)sulfonyl]-2-fluoro[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



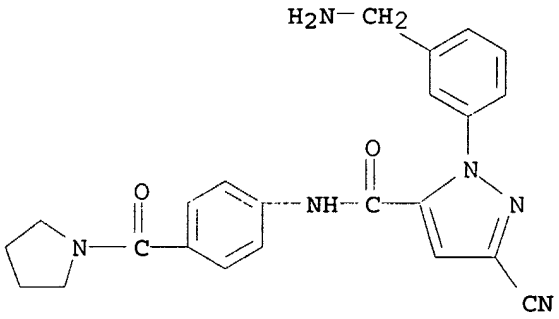
RN 338946-79-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2-fluoro-2'-(1-pyrrolidinylmethyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



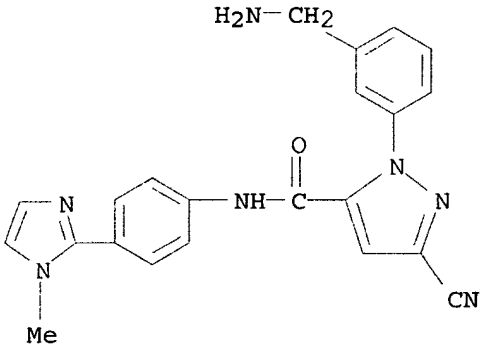
RN 338946-80-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2-fluoro-2'-[(3-hydroxy-1-pyrrolidinyl)methyl][1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



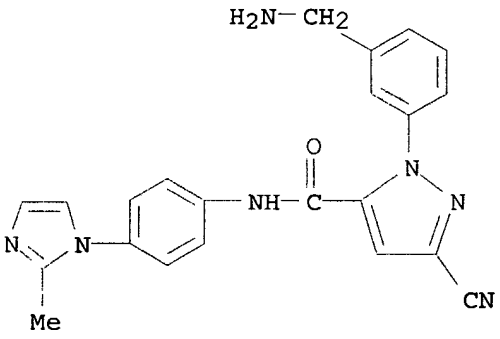
RN 338946-81-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[4-(1-pyrrolidinylcarbonyl)phenyl]- (9CI) (CA INDEX NAME)



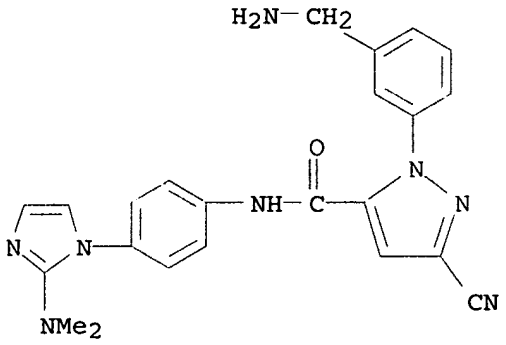
RN 338946-82-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[4-(1-methyl-1H-imidazol-2-yl)phenyl]- (9CI) (CA INDEX NAME)



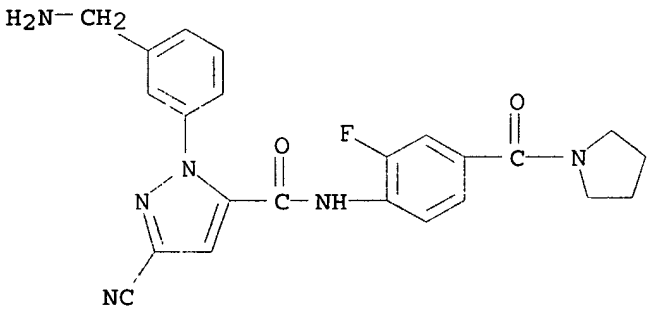
RN 338946-83-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[4-(2-methyl-1H-imidazol-1-yl)phenyl]- (9CI) (CA INDEX NAME)



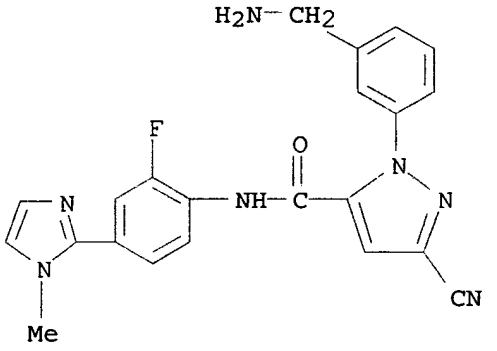
RN 338946-84-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[4-[2-(dimethylamino)-1H-imidazol-1-yl]phenyl]- (9CI) (CA INDEX NAME)



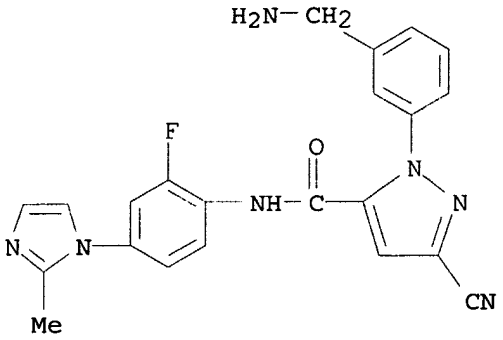
RN 338946-85-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]- (9CI) (CA INDEX NAME)



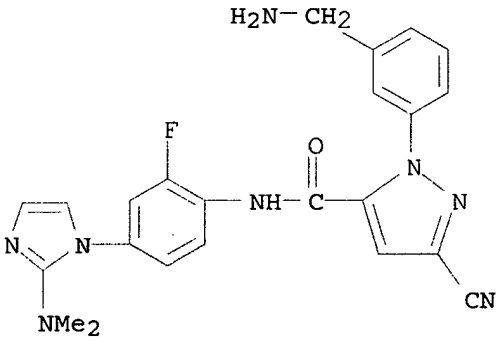
RN 338946-86-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2-fluoro-4-(1-methyl-1H-imidazol-2-yl)phenyl]- (9CI) (CA INDEX NAME)



RN 338946-87-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[2-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]- (9CI) (CA INDEX NAME)



RN 338946-88-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-cyano-N-[4-[2-(dimethylamino)-1H-imidazol-1-yl]-2-fluorophenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

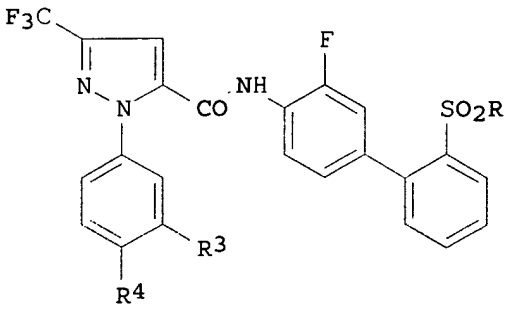
L7 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:300687 CAPLUS
DOCUMENT NUMBER: 134:311206
TITLE: Preparation of 1,3,5-trisubstituted pyrazoles for pharmaceutical use as factor Xa inhibitors
INVENTOR(S): Zhou, Jiacheng; Oh, Lynette May; Confalone, Pasquale N.; Li, Hui-yin; Ma, Philip
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001029006	A1	20010426	WO 2000-US29031	20001020
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				

US 6329527	B1	20011211	US 2000-685127		20001010
CA 2382212	AA	20010426	CA 2000-2382212		20001020
EP 1222172	A1	20020717	EP 2000-972292		20001020
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY					
US 2002055641	A1	20020509	US 2001-5938		20011203
US 6465656	B2	20021015			
PRIORITY APPLN. INFO.:			US 1999-161666P	P	19991021
			US 2000-685127	A3	20001010
			WO 2000-US29031	W	20001020

OTHER SOURCE(S): MARPAT 134:311206

GI



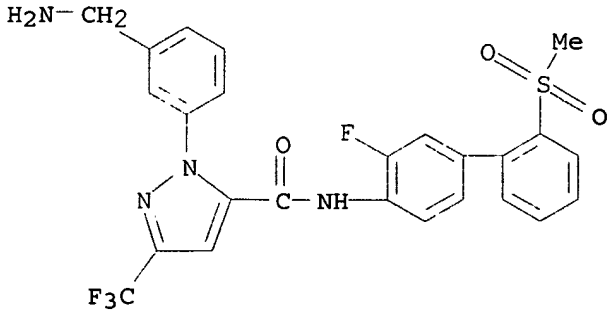
I

AB 1,3,5-Trisubstituted pyrazoles, such as I [R = Me, NH2; R3 = CN, CH2NH2; R4 = H, F], were prepared for pharmaceutical use as factor Xa inhibitors (no biol. testing data presented). Thus, I (R = Me, R3 = CN, R4 = H) was prepared via cyclization of F3CCONHNHC6H4-3-CN with H2C:CHCONHC6H3(-2-F)-4-C6H4-2-SO2Me and subsequent dehydrogenation of the resulting pyrazoline using N-chlorosuccinimide.

IT **292135-59-2P 335275-92-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,3,5-trisubstituted pyrazoles for pharmaceutical use as factor Xa inhibitors)

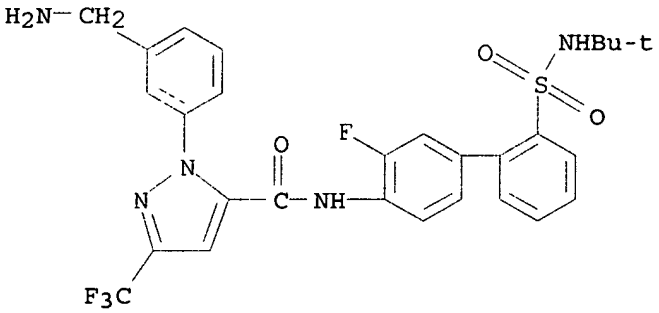
RN 292135-59-2 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 335275-92-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

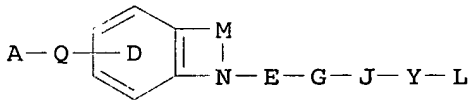
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:137189 CAPLUS
DOCUMENT NUMBER: 134:193446
TITLE: Preparation of heterocyclic compounds as inhibitors of factor Xa
INVENTOR(S): Zhu, Bing-Yan; Scarborough, Robert M.; Clizbe, Lane; Doughan, Brandon; Jia, Zhaozhong-Jon; Kane-Maguire, Kim; Marlowe, Charles; Song, Yonghong; Su, Ting; Teng, Willy; Zhang, Penglie
PATENT ASSIGNEE(S): Cor Therapeutics, Inc., USA; et al.
SOURCE: PCT Int. Appl., 387 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

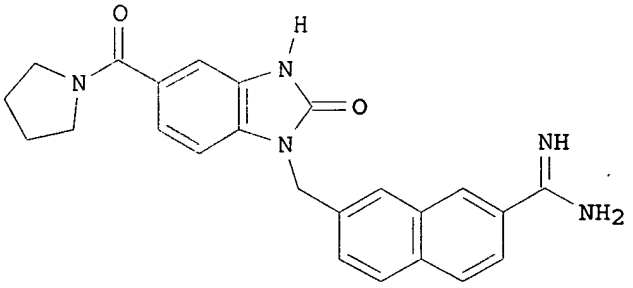
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001012600	A1	20010222	WO 2000-US21742		20000810
WO 2001012600	C2	20020912			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
US 6534535	B1	20030318	US 2000-636804		20000810
PRIORITY APPLN. INFO.:			US 1999-148627P	P	19990812
			US 2000-202202P	P	20000505

OTHER SOURCE(S): MARPAT 134:193446

GI



I



II

AB The title compds. [I; A = alkyl, cycloalkyl, (un)substituted Ph, etc.; Q = a direct link, CH2, CO, etc.; D = (un)substituted Ph, 6-membered heteroaryl having 1-2 ring N atoms; M = NR16CO, NR16CS, CR17R18CO, etc.; R16-R18 = H, halo, alkyl, etc.; E = a direct link, CO, CONR5, etc.; R5 = alkyl, alkenyl, alkynyl, etc.; G = a direct link, CR7R8, CR7aR8aCR7bR8b, CR7c:CR8c; R7, R8, R7a, R7b, R7c, R8a, R8b, R8c = H, halo, alkyl, etc.; J = a direct link, O, S, etc.; Y = (un)substituted Ph, naphthyl, monocyclic or fused bicyclic heterocyclyl; L = H, CN, CONR12R13; R12, R13 = H, alkyl, OH, etc.] having activity against mammalian factor Xa, and useful in vitro or in vivo for preventing or treating coagulation disorders, were prepared and formulated. E.g., a multi-step synthesis of the title compound II was given.

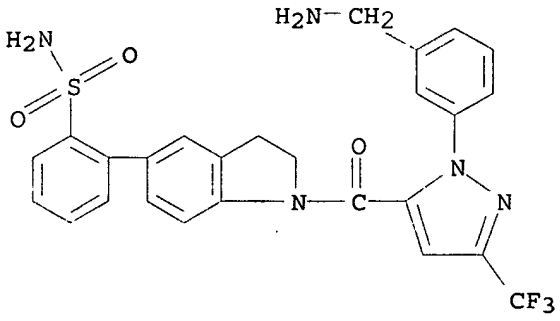
IT **321435-61-4P 327045-28-3P 327046-13-9P 327046-62-8P 327046-63-9P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic compds. as inhibitors of factor Xa)

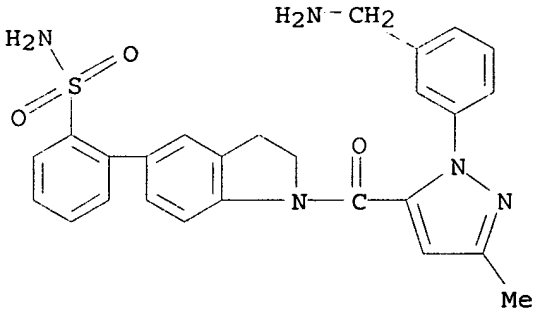
RN 321435-61-4 CAPLUS

CN 1H-Indole, 1-[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]-5-[2-(aminosulfonyl)phenyl]-2,3-dihydro- (9CI) (CA INDEX NAME)



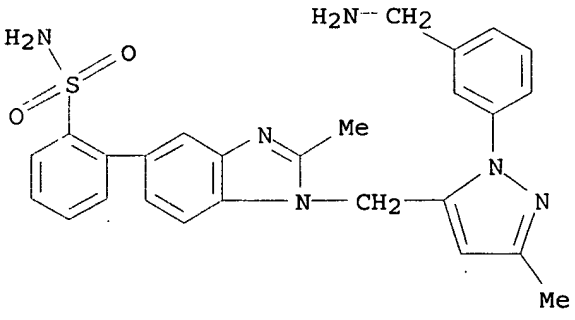
RN 327045-28-3 CAPLUS

CN 1H-Indole, 1-[[1-[3-(aminomethyl)phenyl]-3-methyl-1H-pyrazol-5-yl]carbonyl]-5-[2-(aminosulfonyl)phenyl]-2,3-dihydro- (9CI) (CA INDEX NAME)



RN 327046-13-9 CAPLUS

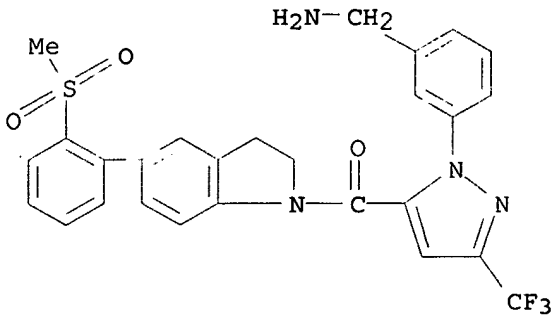
CN Benzenesulfonamide, 2-[1-[[1-[3-(aminomethyl)phenyl]-3-methyl-1H-pyrazol-5-yl]methyl]-2-methyl-1H-benzimidazol-5-yl]- (9CI) (CA INDEX NAME)



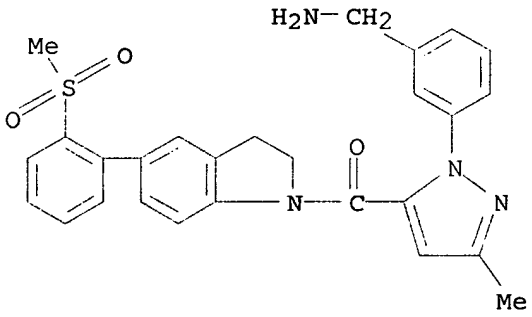
RN 327046-62-8 CAPLUS

CN 1H-Indole, 1-[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]-2,3-dihydro-5-[2-(methylsulfonyl)phenyl]- (9CI) (CA INDEX

NAME)



RN 327046-63-9 CAPLUS
CN 1H-Indole, 1-[[1-[3-(aminomethyl)phenyl]-3-methyl-1H-pyrazol-5-yl]carbonyl]-2,3-dihydro-5-[2-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:63993 CAPLUS
DOCUMENT NUMBER: 134:115952
TITLE: Preparation of nitrogen containing heterobicycles as factor Xa inhibitors
INVENTOR(S): Jacobson, Irina C.; Quan, Mimi L.
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001005784	A1	20010125	WO 2000-US18903	20000712

W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

CA 2380727	AA	20010125	CA 2000-2380727	20000712
EP 1196412	A1	20020417	EP 2000-982716	20000712
EP 1196412	B1	20040609		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000013200	A	20020507	BR 2000-13200	20000712
JP 2004507439	T2	20040311	JP 2001-511443	20000712
AT 268766	E	20040615	AT 2000-982716	20000712
ES 2222257	T3	20050201	ES 2000-982716	20000712
US 6429205	B1	20020806	US 2000-615465	20000713
ZA 2002000094	A	20030218	ZA 2002-94	20020104
NO 2002000217	A	20020315	NO 2002-217	20020115
US 2003096820	A1	20030522	US 2002-205792	20020726
US 6716841	B2	20040406		
HK 1045502	A1	20041210	HK 2002-106604	20020927
PRIORITY APPLN. INFO.:			US 1999-144344P	P 19990716
			WO 2000-US18903	W 20000712
			US 2000-615465	A3 20000713

OTHER SOURCE(S): MARPAT 134:115952
GI

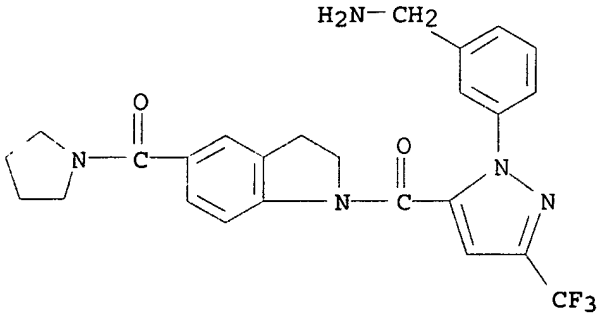
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I or II; G = III, IV (wherein D = (CH2)3, (CH2)4, CH2N:CH; etc.; or ring D is absent; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.); Z = N, CR1a; R1a = absent, (CH2)rR1c, CH:CHR1c, etc.; R1b = absent, (CH2)rR1c, CH:CHR1c, etc.; R1c = H, alkyl, F, etc.; A, A1 = (un)substituted 2-5 membered linker; B = (un)substituted carbocylic residue, 5-10 membered heterocyclic system containing 1-4 heteroatoms, etc.; R4 = H, O, F, etc.; r = 0-3; s = 0-2] which are inhibitors of trypsin-like serine protease enzymes, especially factor Xa, and are useful as anticoagulant agents for treatment and prevention of thromboembolic disorders, were prepared E.g., a multi-step synthesis of the 2,3-dihydro-1H-indole V was given. A number of compds. I or II were found to exhibit a Ki of ≤ 10 μM against factor Xa.

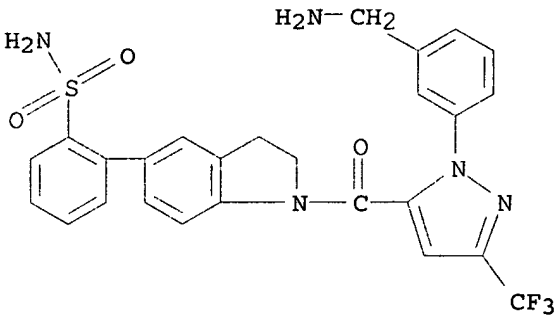
IT **321435-77-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen containing heterobicycles as factor Xa inhibitors)

RN 321435-77-2 CAPLUS

CN 1H-Indole, 1-[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]-2,3-dihydro-5-(1-pyrrolidinylcarbonyl)- (9CI) (CA INDEX NAME)



IT **321435-61-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen containing heterobicycles as factor Xa inhibitors)
RN 321435-61-4 CAPLUS
CN 1H-Indole, 1-[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]-5-[2-(aminosulfonyl)phenyl]-2,3-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

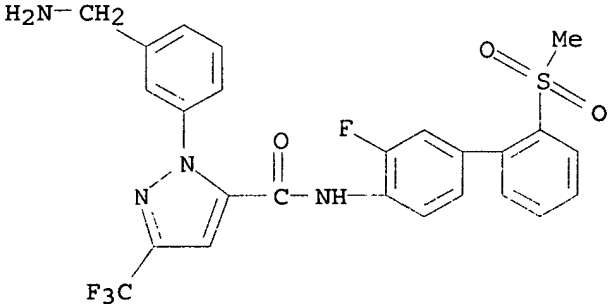
L7 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:705983 CAPLUS
DOCUMENT NUMBER: 136:79226
TITLE: Formation of unusual glutamate conjugates of 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide (DPC 423) and its analogs: the role of γ-glutamyltranspeptidase in the biotransformation of benzylamines
AUTHOR(S): Mutlib, Abdul; Shockcor, John; Chen, Shiang-Yuan; Espina, Robert; Lin, Jianrong; Graciani, Nilsa; Prakash, Shimoga; Gan, Liang-Shang
CORPORATE SOURCE: Drug Metabolism and Pharmacokinetics Section, Stine-Haskell Research Center, DuPont Pharmaceuticals Company, Newark, DE, 19714, USA
SOURCE: Drug Metabolism and Disposition (2001), 29(10), 1296-1306
CODEN: DMDSAI; ISSN: 0090-9556
PUBLISHER: American Society for Pharmacology and Experimental

Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The role of γ-glutamyltranspeptidase (GGT) in transferring glutamate from endogenous glutathione (GSH) to the benzylamine moiety of a compound, such as 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide (DPC 423), is described. Studies were performed with structurally related analogs of DPC 423 to demonstrate that this type of reaction was common to compds. possessing a benzylamine group. Synthesizing appropriate stds. and confirming by liquid chromatog. (LC)/mass spectroscopy and LC/NMR made unambiguous assignments of the structures of glutamate conjugates of DPC 423. The use of stable isotope-labeled GSH for metabolism studies has not been described before. In the present study, we report the novel use of deuterated GSH in conjunction with mass spectral anal. to demonstrate the glutamate transfer to the benzylamines in the presence of GGT. To further demonstrate that the α protons on the benzylamines and glutamate (as part of glutathione) were unaffected during the transpeptidation, these protons were replaced with deuterium. Acivicin (AT-125), a potent and selective inhibitor of GGT, was used to abolish the formation of the glutamate conjugates of DPC 423 in vitro and in vivo. This provided further evidence of the role of GGT in forming the glutamate conjugates of benzylamines. This study demonstrated conclusively that GGT was responsible for mediating the transfer of glutamic acid from GSH to the benzylamine moiety of a series of structurally related compds.

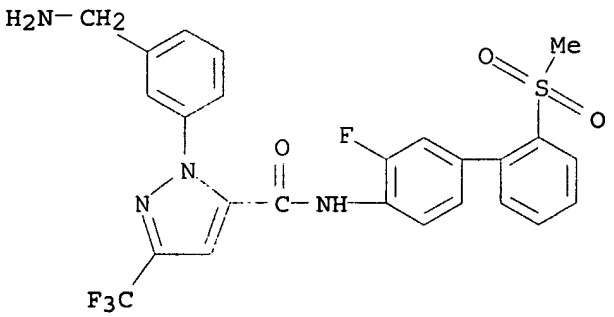
IT **292135-59-2**, DPC 423 **292135-59-2D**, DPC 423, glutamate conjugates
RL: PKT (Pharmacokinetics); BIOL (Biological study)
(formation of unusual glutamate conjugates of DPC 423 and its analogs and role of γ-glutamyltranspeptidase in the biotransformation of benzylamines)

RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:55833 CAPLUS
DOCUMENT NUMBER: 134:246871
TITLE: Discovery of 1-[3-(Aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide (DPC423), a Highly Potent, Selective, and Orally Bioavailable Inhibitor of Blood Coagulation Factor Xa
AUTHOR(S): Pinto, Donald J. P.; Orwat, Michael J.; Wang, Shuaige; Fevig, John M.; Quan, Mimi L.; Amparo, Eugene; Cacciola, Joseph; Rossi, Karen A.; Alexander, Richard S.; Smallwood, Angela M.; Luettgen, Joseph M.; Liang, Li; Aungst, Bruce J.; Wright, Matthew R.; Knabb, Robert M.; Wong, Pancras C.; Wexler, Ruth R.; Lam, Patrick Y. S.
CORPORATE SOURCE: DuPont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(4), 566-578
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:246871

AB Factor Xa (fXa) plays a critical role in the coagulation cascade, serving as the point of convergence of the intrinsic and extrinsic pathways. Together with nonenzymic cofactor Va and Ca2+ on the phospholipid surface of platelets or endothelial cells, factor Xa forms the prothrombinase complex, which is responsible for the proteolysis of prothrombin to catalytically active thrombin. Thrombin, in turn, catalyzes the cleavage of fibrinogen to fibrin, thus initiating a process that ultimately leads to clot formation. Recently, the authors reported on a series of isoxazoline and isoxazole monobasic noncovalent inhibitors of factor Xa which show good potency in animal models of thrombosis. In this paper, the authors wish to report on the optimization of the heterocyclic core, which ultimately led to the discovery of a novel pyrazole SN429 (fXa Ki = 13 pM). The authors also report on the authors efforts to improve the oral bioavailability and pharmacokinetic profile of this series while maintaining subnanomolar potency and in vitro selectivity. This was achieved by replacing the highly basic benzamidine P1 with a less basic benzylamine moiety. Further optimization of the pyrazole core

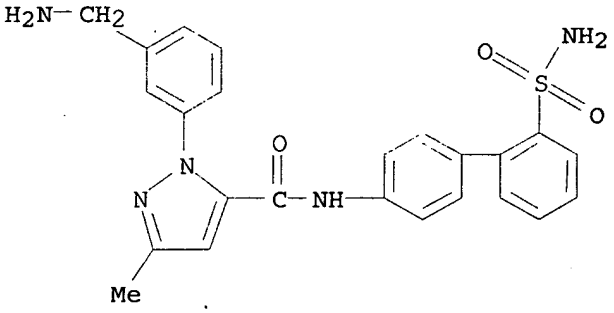
substitution and the biphenyl P4 culminated in the discovery of DPC423, a highly potent, selective, and orally active factor Xa inhibitor which was chosen for clin. development.

IT **209955-59-9P 209955-61-3P 209957-34-6P 209957-36-8P 209957-48-2P 209957-66-4P 209957-76-6P 209957-78-8P 292135-59-2P**, DPC 423
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(discovery of pyrazolecarboxamide derivative (DPC423) as a highly potent and orally bioavailable inhibitor of blood coagulation factor Xa with good pharmacokinetics and structure-activity relationships)

RN 209955-59-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

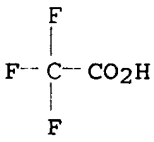
CM 1

CRN 209955-58-8
CMF C24 H23 N5 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

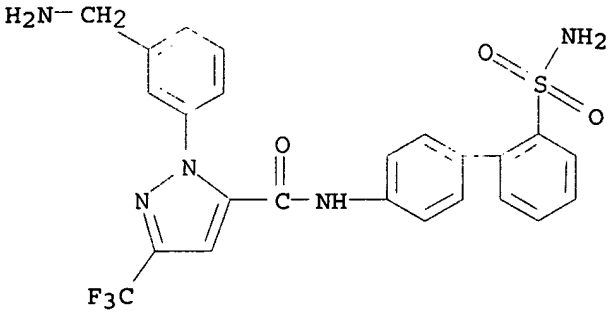


RN 209955-61-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

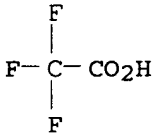
CRN 209955-60-2

CMF C24 H20 F3 N5 O3 S



CM 2

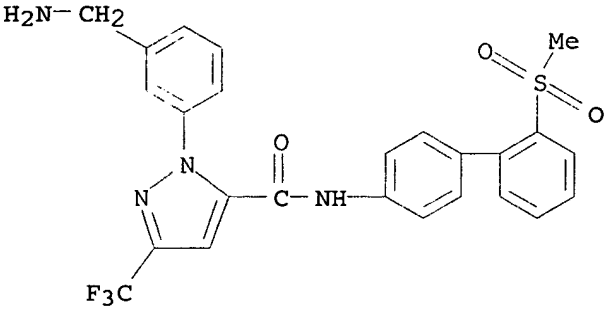
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-34-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

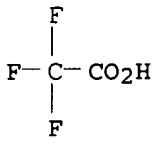
CM 1

CRN 209957-33-5
CMF C25 H21 F3 N4 O3 S



CM 2

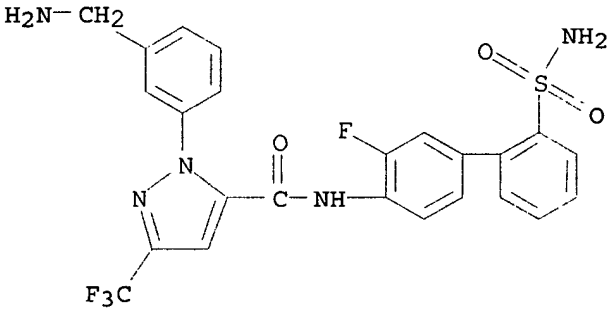
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-36-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

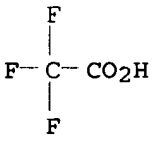
CM 1

CRN 209957-35-7
CMF C24 H19 F4 N5 O3 S



CM 2

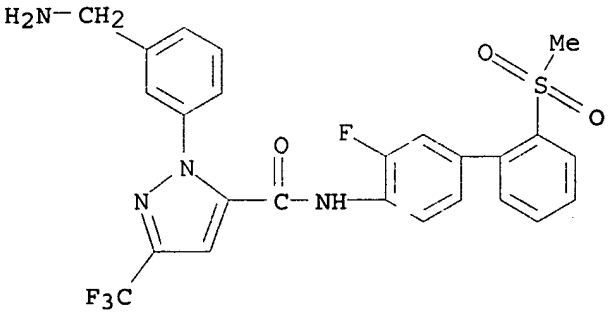
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-48-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

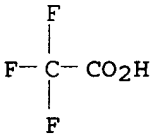
CM 1

CRN 209957-47-1
CMF C25 H20 F4 N4 O3 S



CM 2

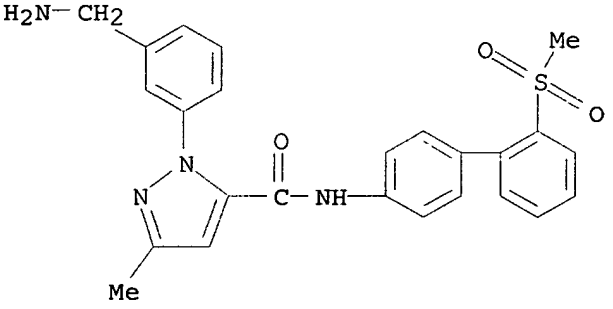
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-66-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-methyl-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

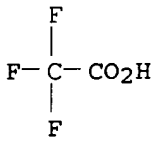
CM 1

CRN 209957-65-3
CMF C25 H24 N4 O3 S



CM 2

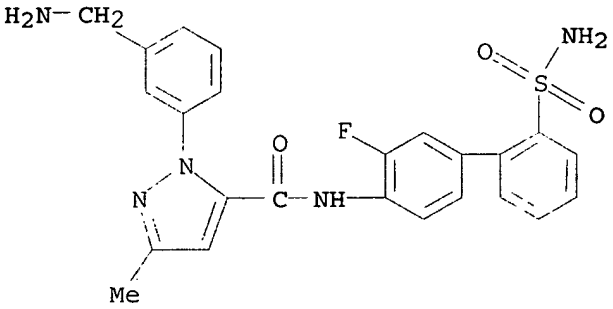
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-76-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

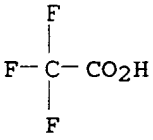
CM 1

CRN 209957-75-5
CMF C24 H22 F N5 O3 S



CM 2

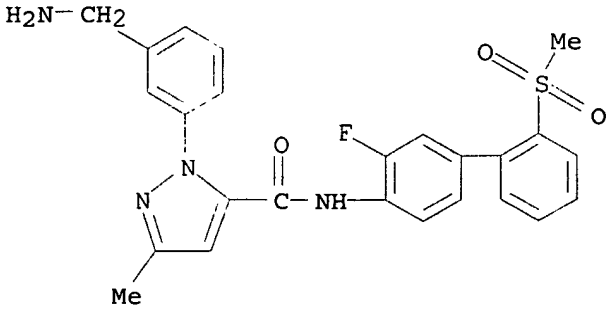
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-78-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

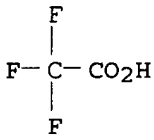
CM 1

CRN 209957-77-7
CMF C25 H23 F N4 O3 S

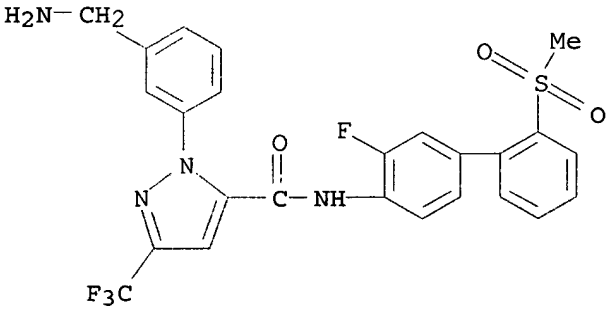


CM 2

CRN 76-05-1
CMF C2 H F3 O2



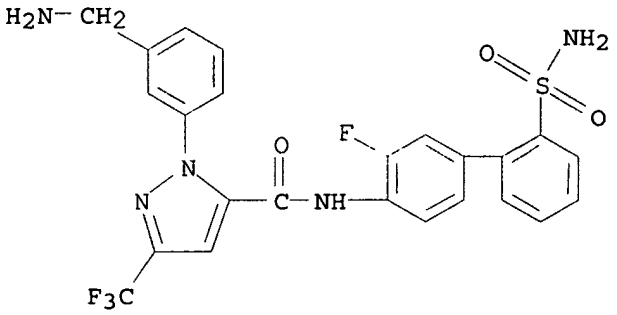
RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT **209957-35-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(discovery of pyrazolecarboxamide derivative (DPC423) as a highly potent and orally bioavailable inhibitor of blood coagulation factor Xa with good pharmacokinetics and structure-activity relationships)
RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-

3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



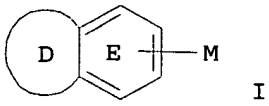
REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:725629 CAPLUS
DOCUMENT NUMBER: 133:296430
TITLE: Preparation of aryl sulfonyls as factor Xa inhibitors
INVENTOR(S): Wexler, Ruth R.; Jacobson, Irina C.
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000059902	A2	20001012	WO 2000-US8364	20000330
WO 2000059902	A3	20010426		
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2368630	AA	20001012	CA 2000-2368630	20000330
EP 1175419	A2	20020130	EP 2000-923096	20000330
EP 1175419	B1	20030528		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 241621	E	20030615	AT 2000-923096	20000330
ES 2197092	T3	20040101	ES 2000-923096	20000330
US 6399644	B1	20020604	US 2000-540467	20000331
US 2003050315	A1	20030313	US 2002-74301	20020212
US 6689770	B2	20040210		

PRIORITY APPLN. INFO.:	US 1999-127634P	P	19990402
	WO 2000-US8364	W	20000330
	US 2000-540467	A3	20000331

OTHER SOURCE(S): MARPAT 133:296430
GI



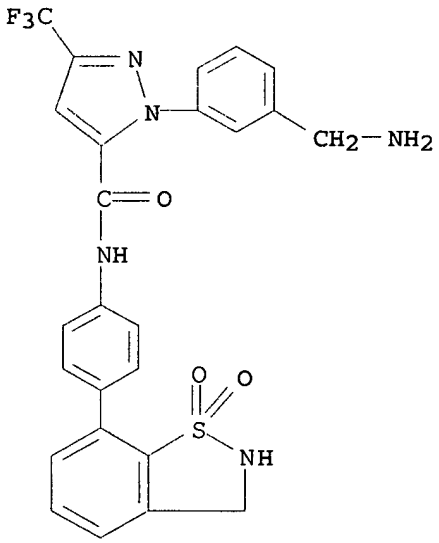
I

AB Aryl sulfonyls I [ring D is absent or is CH2N:CH, CH:NCH2, aromatic system containing heteroatoms, etc.; E = Ph, pyridyl, pyrazinyl, etc.; M = heterocyclyl], effective factor Xa inhibitors (no data), were prepared E.g., N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-1-(4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide was prepared

IT **300710-16-1P 300710-17-2P 300710-18-3P 300710-24-1P 300710-28-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryl sulfonyls as factor Xa inhibitors)

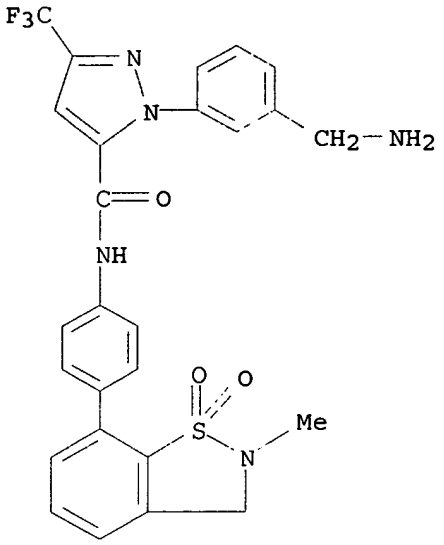
RN 300710-16-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

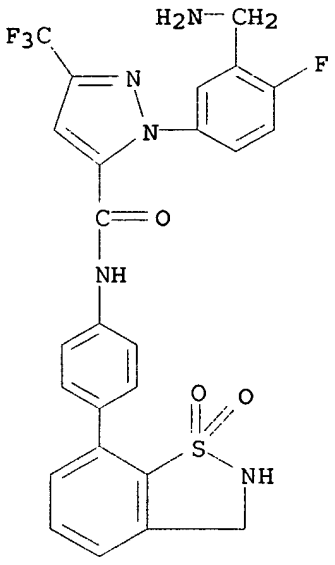


RN 300710-17-2 CAPLUS

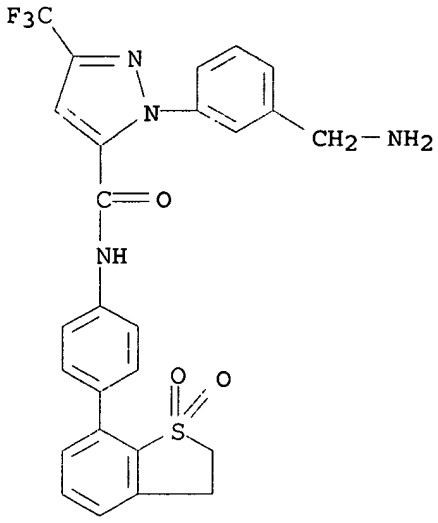
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



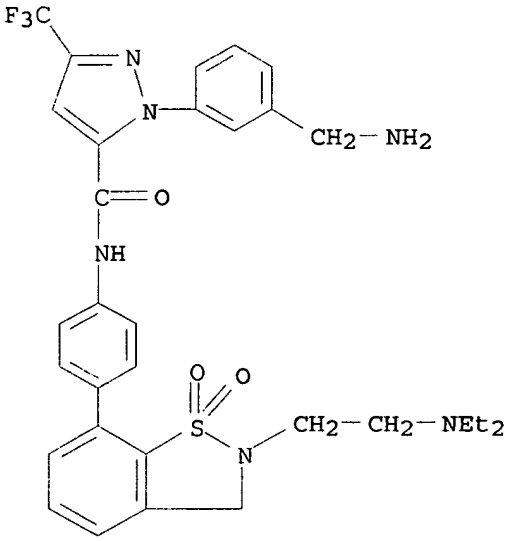
RN 300710-18-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



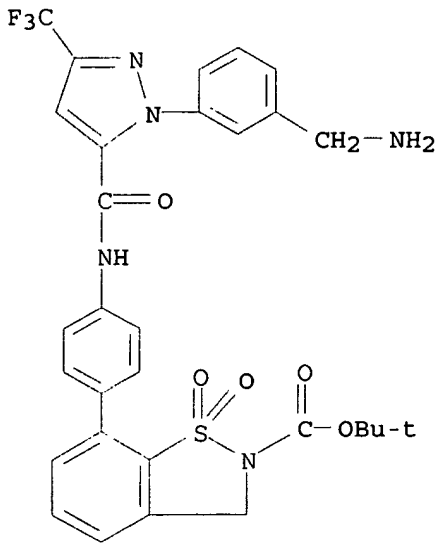
RN 300710-24-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxidobenzo[b]thien-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 300710-28-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[2-[2-(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT **300710-45-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl sulfonyls as factor Xa inhibitors)
RN 300710-45-6 CAPLUS
CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-[[[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

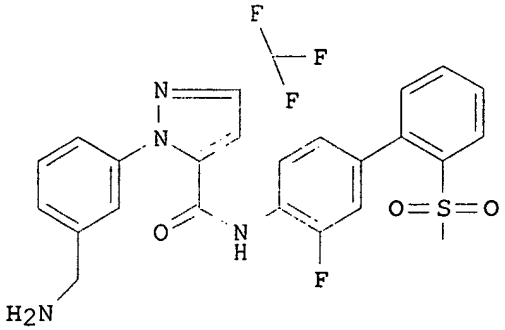


L7 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:645898 CAPLUS
DOCUMENT NUMBER: 133:232835
TITLE: Treatment of thrombosis by combined use of a factor xa inhibitor and aspirin, tissue plasminogen activator (TPA), a GPIIb/IIIa antagonist, low molecular weight heparin or heparin
INVENTOR(S): Wong, Pancras C.
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000053264	A1	20000914	WO 2000-US6451	20000310
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6794412	B1	20040921	US 2000-519188	20000306
CA 2361650	AA	20000914	CA 2000-2361650	20000310
EP 1161279	A1	20011212	EP 2000-913894	20000310
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000010381	A	20020205	BR 2000-10381	20000310
AU 766089	B2	20031009	AU 2000-35254	20000310
NZ 513217	A	20031128	NZ 2000-513217	20000310
ZA 2001006360	A	20020802	ZA 2001-6360	20010802

PRIORITY APPLN. INFO.:	US 1999-123815P	P	19990311
	WO 2000-US6451	W	20000310

GI



I

AB Provided is a method of treating thrombosis in mammals by administering therapeutically effective amts. of a combination of (i) a Factor Xa inhibitor, and (ii) a compound selected from the group consisting of aspirin, TPA, a GPIIb/IIIa antagonist, low mol. weight heparin and heparin, wherein the dose administered for at least one of (i) and (ii) is a subtherapeutic dose. Preferably, the combination of (i) and (ii) provides a synergistic effect. A combination of I (Factor Xa inhibitor) and aspirin at their subtherapeutic doses produced a significant antithrombotic effect in a rabbit model of arterial thrombosis. Pharmaceutical dosage forms are discussed.

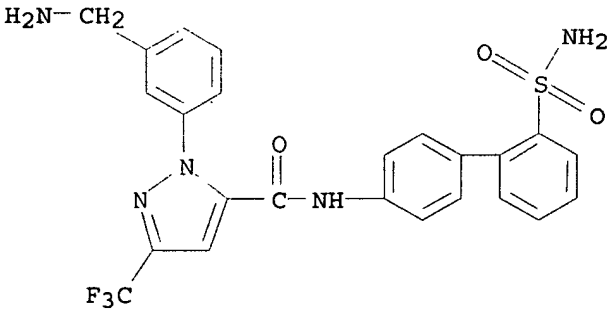
IT **209955-61-3 209957-48-2 292135-59-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antithrombotic combination of a Factor Xa inhibitor and aspirin, TPA, a GPIIb/IIIa antagonist, or heparin derivative)

RN 209955-61-3 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

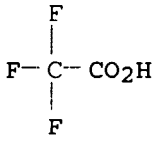
CM 1

CRN 209955-60-2
CMF C24 H20 F3 N5 O3 S



CM 2

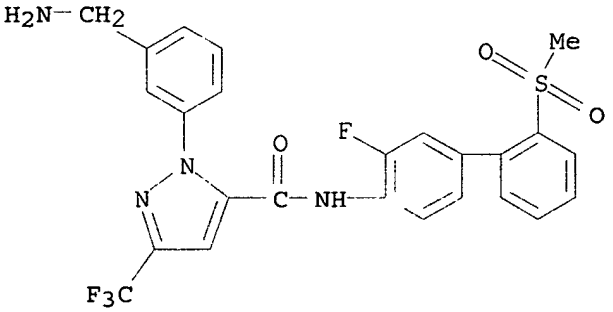
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-48-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

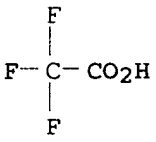
CM 1

CRN 209957-47-1
CMF C25 H20 F4 N4 O3 S

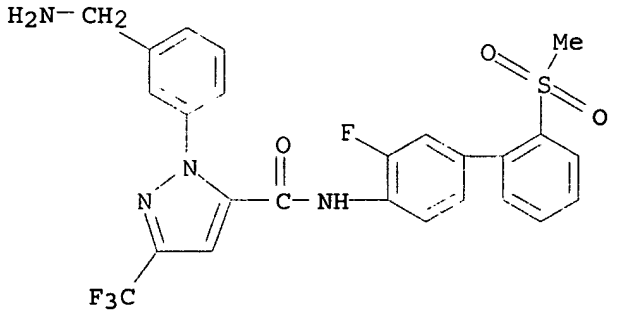


CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

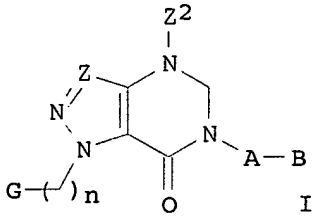
L7 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:457072 CAPLUS
DOCUMENT NUMBER: 133:74031
TITLE: Preparation of nitrogen-containing heterobicycles [pyrazolopyrimidines and analogs] as factor Xa inhibitors
INVENTOR(S): Fevig, John M.; Cacciola, Joseph; Clark, Charles G.; Lam, Patrick Yuk Sun; Pinto, Donald J. P.; Pruitt, James R.; Rossi, Karen A.
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 333 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000039131	A1	20000706	WO 1999-US30316	19991217
W: AL, AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MK, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2349330	AA	20000706	CA 1999-2349330	19991217
EP 1140941	A1	20011010	EP 1999-967444	19991217
EP 1140941	B1	20041020		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9917080	A	20020312	BR 1999-17080	19991217
AU 759711	B2	20030417	AU 2000-23717	19991217
NZ 511674	A	20031128	NZ 1999-511674	19991217
AT 280171	E	20041115	AT 1999-967444	19991217
PT 1140941	T	20050228	PT 1999-967444	19991217
ES 2232202	T3	20050516	ES 1999-967444	19991217
HR 990396	A1	20000831	HR 1999-990396	19991221
TW 225862	B1	20050101	TW 1999-88122748	20000115
ZA 2001003795	A	20020812	ZA 2001-3795	20010510

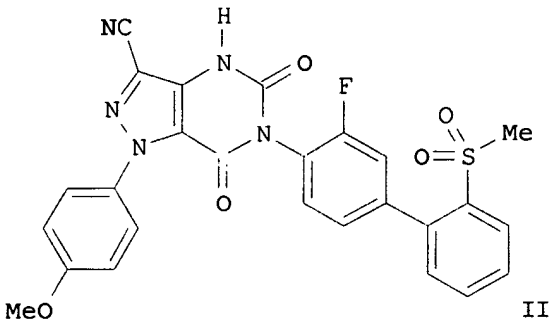
NO 2001003072	A	20010620	NO 2001-3072		20010620
NO 319816	B1	20050919			
PRIORITY APPLN. INFO.:			US 1998-113628P	P	19981223
			US 1999-127633P	P	19990402
			WO 1999-US30316	W	19991217

OTHER SOURCE(S): MARPAT 133:74031

GI



I



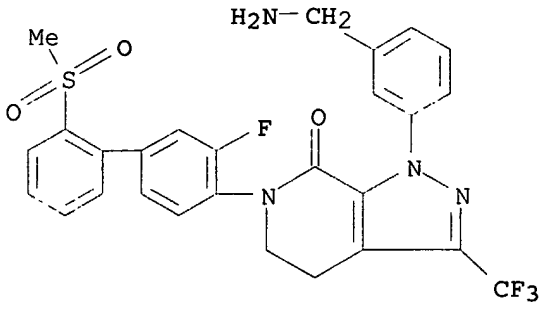
II

AB The application describes nitrogen-containing heterobicyclics and derivs., or their pharmaceutically acceptable salt forms, which are useful as inhibitors of factor Xa. In particular, compds. belonging to 66 generalized structures, such as I, are claimed [wherein the rings may bear 0-2 alkyl or Ph substituents; G = variety of (un)substituted mono- and bicyclic derivs. of Ph, pyridyl, pyrimidyl, etc.; n = 0-2; Z = N or (un)substituted CH; Z2 = H, alkyl, Ph, PhCH2, acyl, or alkyl- or phenylthio, -sulfinyl, or -sulfonyl; A = carbocyclyl or N/O/S-heterocyclyl; B = variety of substituents, notably various kinds of amino-group-containing substituents, or (un)substituted carbocyclyl or heterocyclyl]. Over 100 invention compound examples, mostly as salts, are given, and the free base forms are claimed. For instance, condensation of 4-anisidine with malononitrile (97%) and cyclization with Me bromoacetate (34%) gave Me 1-(4-methoxyphenyl)-3-cyano-4-aminopyrazole-5-carboxylate. The latter compound underwent diazotization and protection of the amine as an azide (57%), amidation with a biphen-4-ylamine derivative (5%), reduction of the azide to an amine (19%), and cyclization with carbonyldiimidazole (11%), to give title compound II. Selected compds. I inhibited factor Xa in vitro with Ki ≤ 10 μM, and some compds. inhibited thrombin in vitro with Ki < 10 μM.

IT **280118-38-9P 280118-39-0P 280119-05-3P**
280119-06-4P 280119-07-5P 280119-08-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of pyrazolopyrimidinones and other N-containing heterobicyclics as factor Xa and thrombin inhibitors)

RN 280118-38-9 CAPLUS

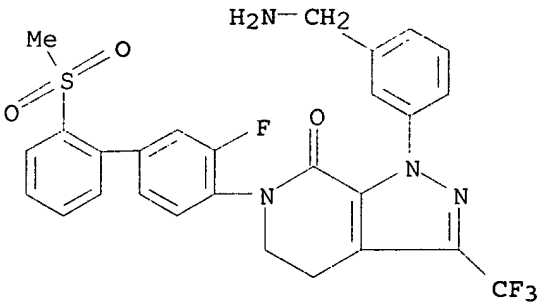
CN 7H-Pyrazolo[3,4-c]pyridin-7-one, 1-[3-(aminomethyl)phenyl]-6-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1,4,5,6-tetrahydro-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 280118-39-0 CAPLUS
CN 7H-Pyrazolo[3,4-c]pyridin-7-one, 1-[3-(aminomethyl)phenyl]-6-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1,4,5,6-tetrahydro-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

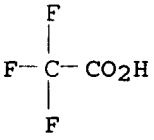
CM 1

CRN 280118-38-9
CMF C27 H22 F4 N4 O3 S



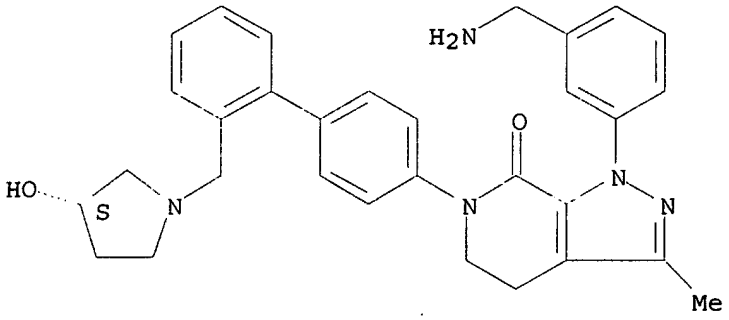
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 280119-05-3 CAPLUS
CN 7H-Pyrazolo[3,4-c]pyridin-7-one, 1-[3-(aminomethyl)phenyl]-1,4,5,6-tetrahydro-6-[2'-[[(3S)-3-hydroxy-1-pyrrolidinyl]methyl][1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

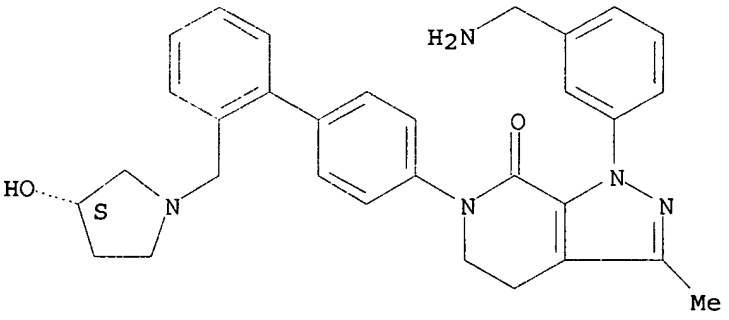


RN 280119-06-4 CAPLUS
CN 7H-Pyrazolo[3,4-c]pyridin-7-one, 1-[3-(aminomethyl)phenyl]-1,4,5,6-tetrahydro-6-[2'-[[(3S)-3-hydroxy-1-pyrrolidinyl]methyl][1,1'-biphenyl]-4-yl]-3-methyl-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

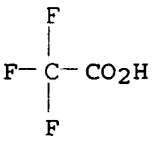
CRN 280119-05-3
CMF C31 H33 N5 O2

Absolute stereochemistry.

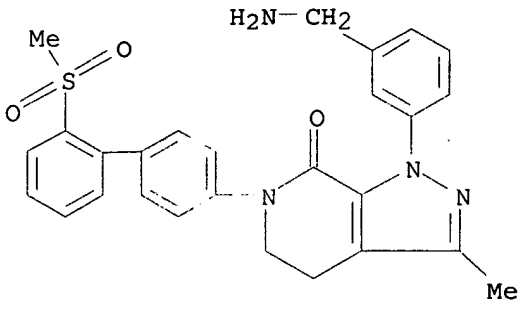


CM 2

CRN 76-05-1
CMF C2 H F3 O2



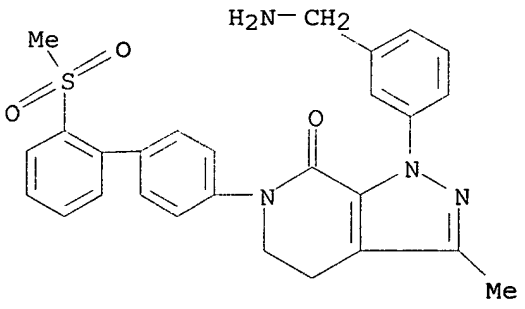
RN 280119-07-5 CAPLUS
CN 7H-Pyrazolo[3,4-c]pyridin-7-one, 1-[3-(aminomethyl)phenyl]-1,4,5,6-tetrahydro-3-methyl-6-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 280119-08-6 CAPLUS
CN 7H-Pyrazolo[3,4-c]pyridin-7-one, 1-[3-(aminomethyl)phenyl]-1,4,5,6-tetrahydro-3-methyl-6-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

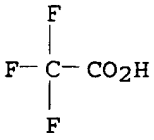
CM 1

CRN 280119-07-5
CMF C27 H26 N4 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2



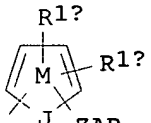
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:83115 CAPLUS
DOCUMENT NUMBER: 132:137392
TITLE: Preparation of azoles as Factor Xa inhibitors.
INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell;

Cacciola, Joseph; Fevig, John Matthew; Han, Qi; Orwat, Michael James; Quan, Mimi Lifen; Rossi, Karen Anita
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Co., USA
SOURCE: U.S., 152 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 6020357	A	20000201	US 1997-995834		19971222
US 6548512	B1	20030415	US 2000-492708		20000127
PRIORITY APPLN. INFO.:			US 1996-33437P	P	19961223
			US 1997-50304P	P	19970620
			US 1997-995834	A3	19971222

OTHER SOURCE(S): MARPAT 132:137392
GI

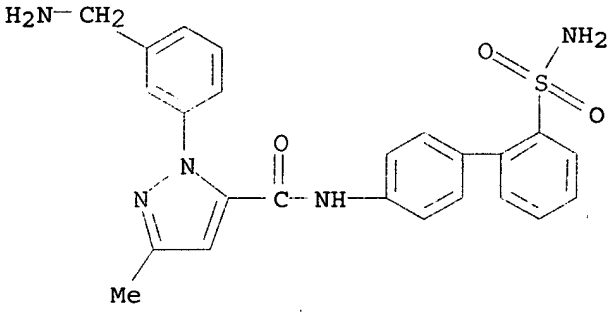


I

AB Title compds. [I; ring M contains, in addition to J, 0-3 N atoms; J = N, NH; D = CN, C(:NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G = absent, NHCH2, OCH2, etc.; Z = C1-4 alkylene, (CH2)rO(CH2)r, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, C1-6 alkyl, etc.; R8, R9 = H, C1-6 alkyl, (CH2)nPh; n = 0-3; r = 0-3; s = 0-2; with provisos], useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-[o-(tert-BuSO2)phenyl]aniline with Me3Al/hexane in CH2Cl2 followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the Pinner reaction of the resulting intermediate afforded 1-(3-amidinophenyl)-2-[(2'-aminosulfonyl-1,1'-biphen-4-yl)aminocarbonyl]imidazole. Several I showed Ki ≤10 μM against Factor Xa and thrombin.
IT **209955-58-8P 209955-59-9P 209955-60-2P**
209955-61-3P 209956-42-3P 209956-93-4P
209956-94-5P 209956-95-6P 209956-96-7P
209956-97-8P 209956-98-9P 209956-99-0P
209957-00-6P 209957-27-7P 209957-28-8P
209957-29-9P 209957-30-2P 209957-31-3P
209957-32-4P 209957-33-5P 209957-34-6P
209957-35-7P 209957-36-8P 209957-38-0P
209957-40-4P 209957-45-9P 209957-46-0P
209957-47-1P 209957-48-2P 209957-50-6P
209957-55-1P 209957-56-2P 209957-57-3P
209957-58-4P 209957-61-9P 209957-65-3P
209957-66-4P 209957-67-5P 209957-68-6P
209957-71-1P 209957-72-2P 209957-73-3P

209957-74-4P 209957-75-5P 209957-76-6P
209957-81-3P 209957-83-5P 209957-92-6P
209957-93-7P 209957-94-8P 209957-95-9P
209957-96-0P 209957-97-1P 209957-98-2P
209957-99-3P 209958-07-6P 209958-08-7P
209958-09-8P 209958-10-1P 209958-11-2P
209958-12-3P 209958-13-4P 209958-14-5P
209958-15-6P 209958-16-7P 209958-17-8P
209958-18-9P 209958-19-0P 209958-20-3P
209958-21-4P 209958-22-5P 209958-24-7P
209958-25-8P 209958-26-9P 209958-27-0P
209958-28-1P 209958-29-2P 209958-30-5P
209958-31-6P 256512-27-3P 256512-29-5P
256512-30-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azoles as Factor Xa inhibitors)

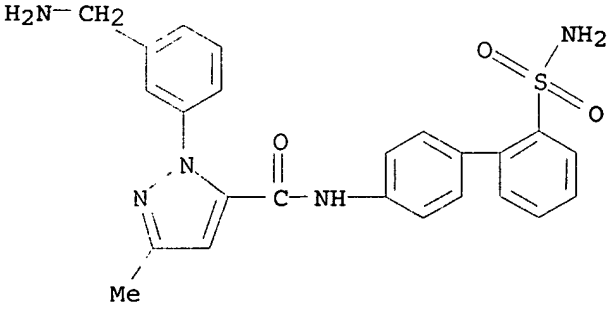
RN 209955-58-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209955-59-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

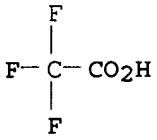
CM 1

CRN 209955-58-8
CMF C24 H23 N5 O3 S

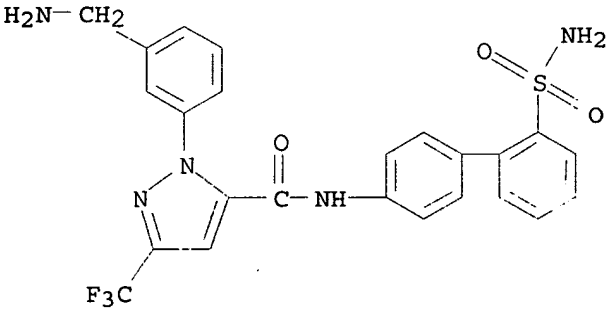


CM 2

CRN 76-05-1
CMF C2 H F3 O2



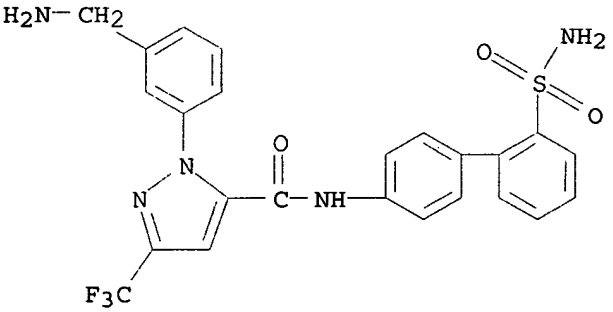
RN 209955-60-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-61-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

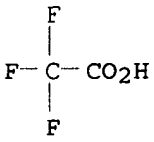
CM 1

CRN 209955-60-2
CMF C24 H20 F3 N5 O3 S

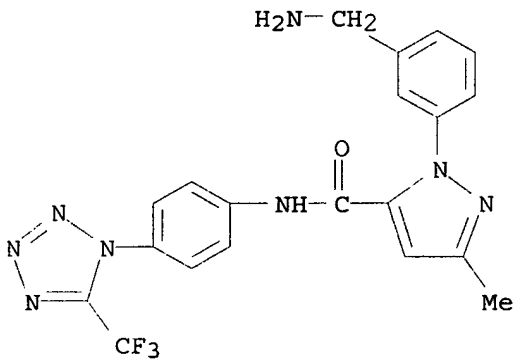


CM 2

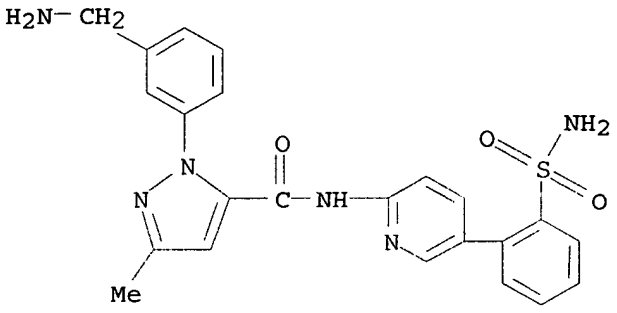
CRN 76-05-1
CMF C2 H F3 O2



RN 209956-42-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-methyl-N-[4-[5-(trifluoromethyl)-1H-tetrazol-1-yl]phenyl]- (9CI) (CA INDEX NAME)



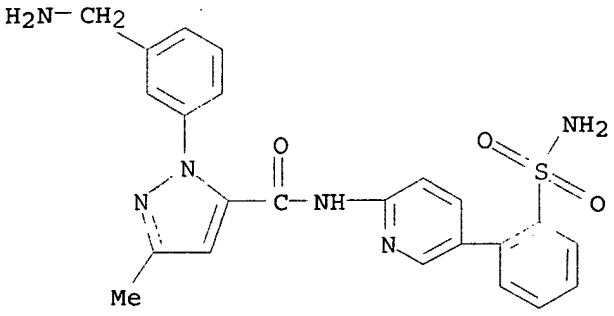
RN 209956-93-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209956-94-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

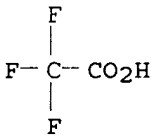
CM 1

CRN 209956-93-4
CMF C23 H22 N6 O3 S

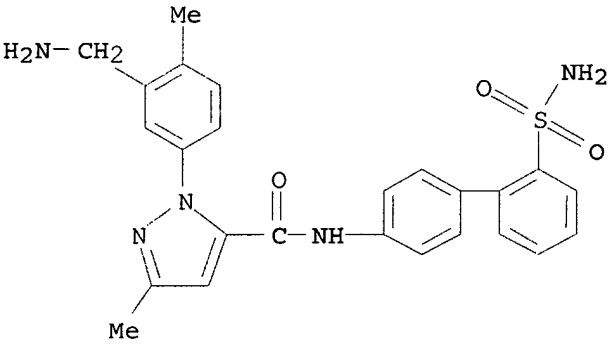


CM 2

CRN 76-05-1
CMF C2 H F3 O2



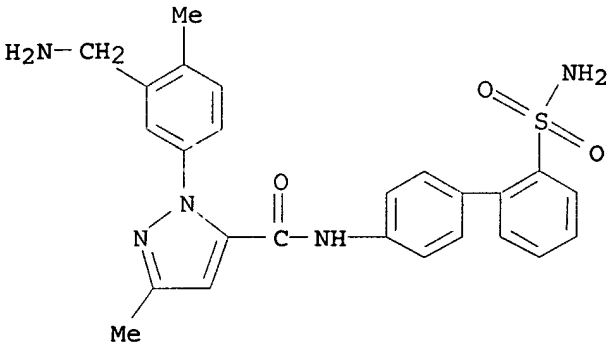
RN 209956-95-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-methylphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209956-96-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-methylphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

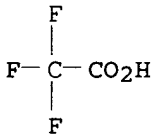
CM 1

CRN 209956-95-6
CMF C25 H25 N5 O3 S

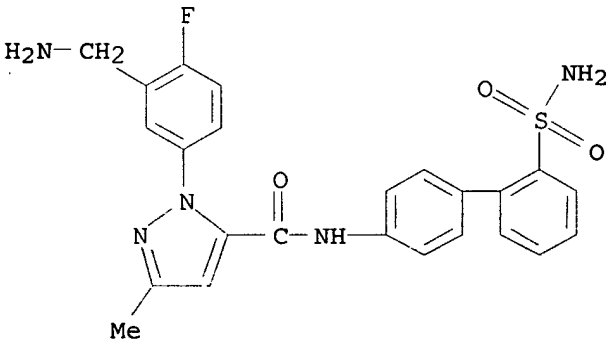


CM 2

CRN 76-05-1
CMF C2 H F3 O2



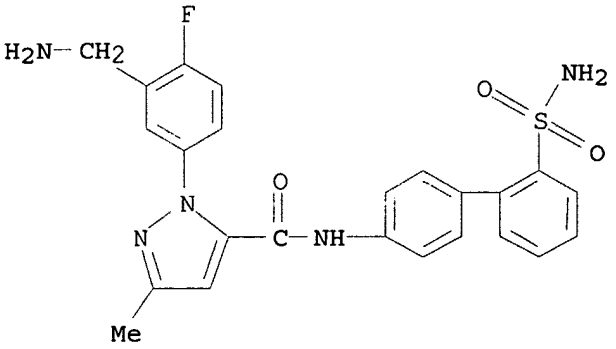
RN 209956-97-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209956-98-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

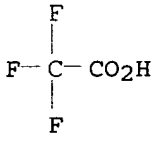
CM 1

CRN 209956-97-8
CMF C24 H22 F N5 O3 S

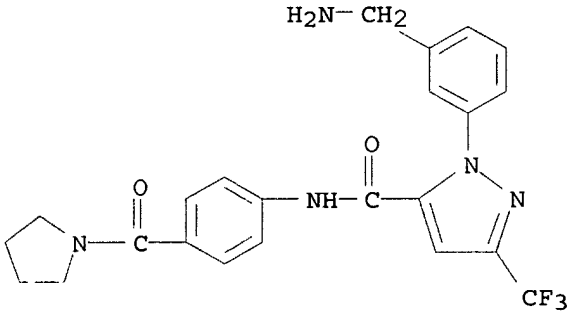


CM 2

CRN 76-05-1
CMF C2 H F3 O2



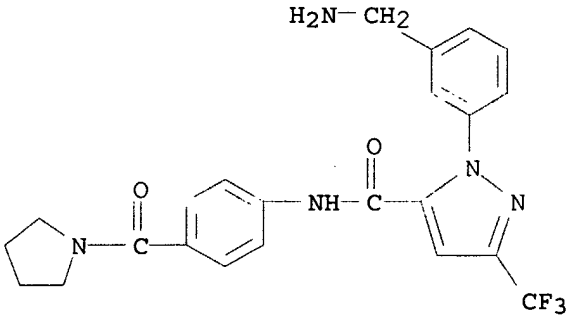
RN 209956-99-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-00-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

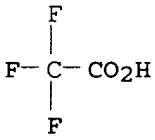
CM 1

CRN 209956-99-0
CMF C23 H22 F3 N5 O2

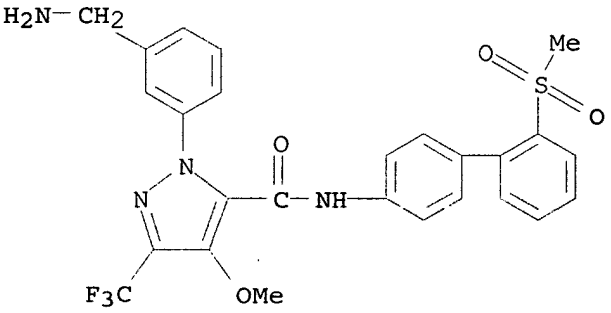


CM 2

CRN 76-05-1
CMF C2 H F3 O2



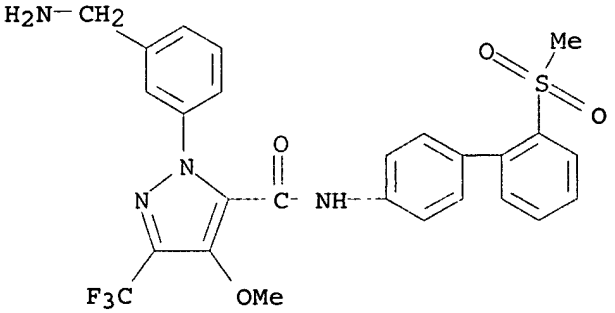
RN 209957-27-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-28-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

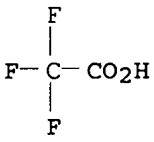
CM 1

CRN 209957-27-7
CMF C26 H23 F3 N4 O4 S

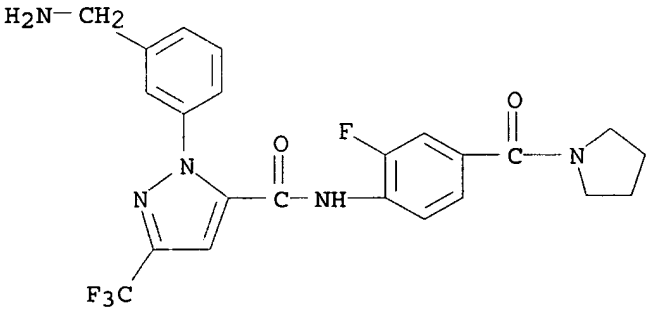


CM 2

CRN 76-05-1
CMF C2 H F3 O2



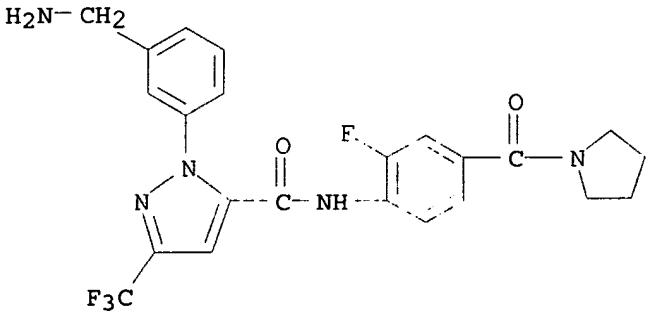
RN 209957-29-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-30-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

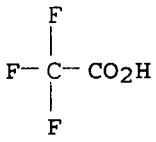
CM 1

CRN 209957-29-9
CMF C23 H21 F4 N5 O2

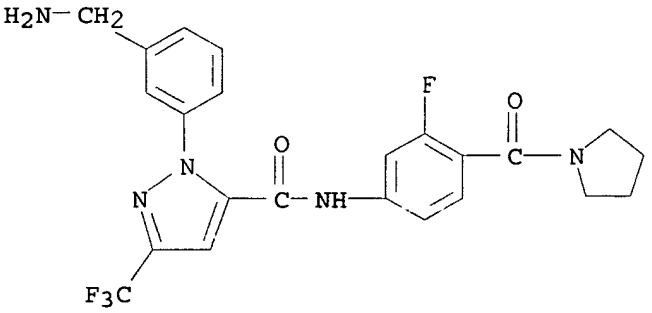


CM 2

CRN 76-05-1
CMF C2 H F3 O2



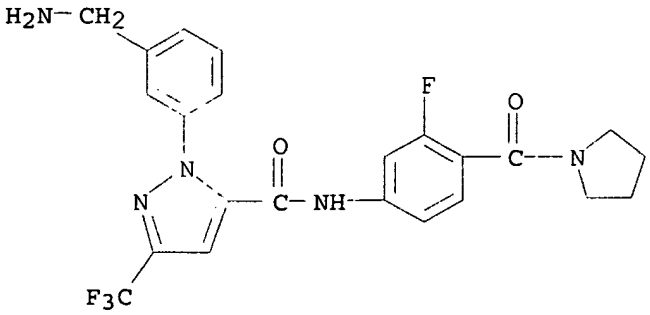
RN 209957-31-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-32-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

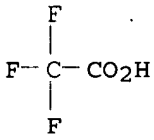
CM 1

CRN 209957-31-3
CMF C23 H21 F4 N5 O2

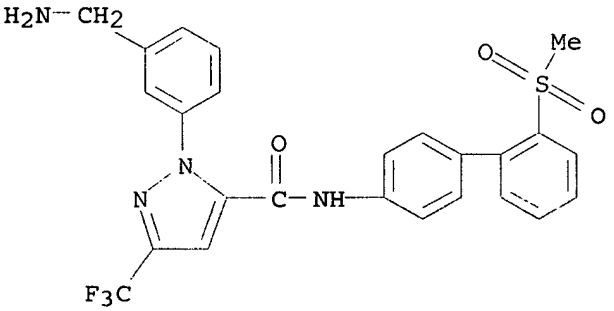


CM 2

CRN 76-05-1
CMF C2 H F3 O2



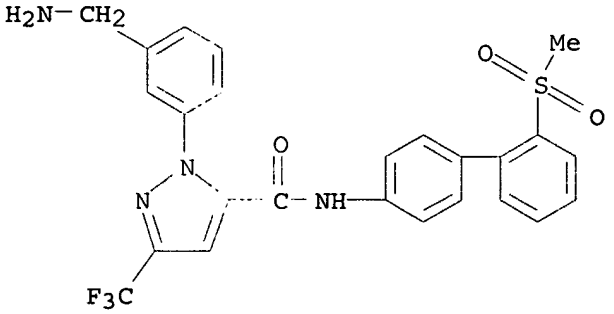
RN 209957-33-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-34-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

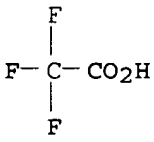
CM 1

CRN 209957-33-5
CMF C25 H21 F3 N4 O3 S

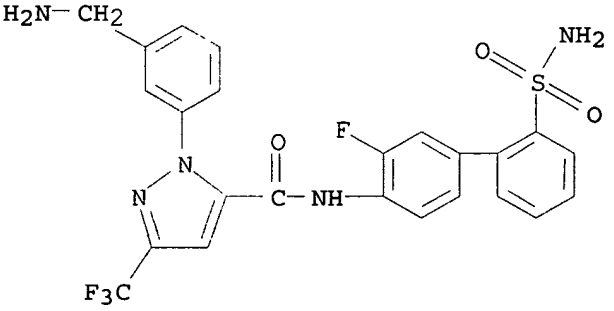


CM 2

CRN 76-05-1
CMF C2 H F3 O2



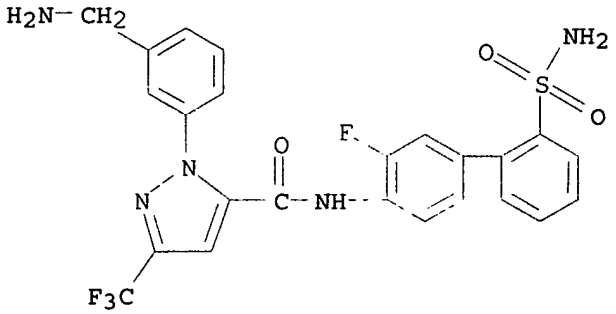
RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-36-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

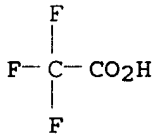
CM 1

CRN 209957-35-7
CMF C24 H19 F4 N5 O3 S



CM 2

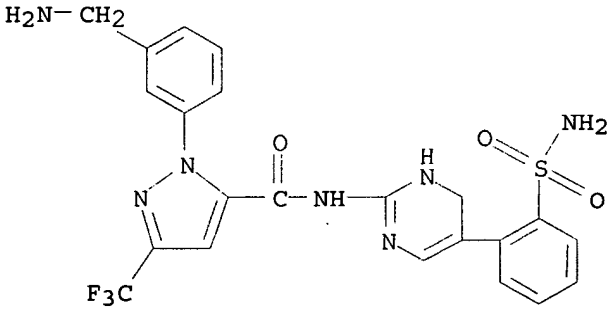
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-38-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-1,4-dihydro-2-pyrimidinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

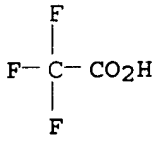
CM 1

CRN 209957-37-9
CMF C22 H20 F3 N7 O3 S



CM 2

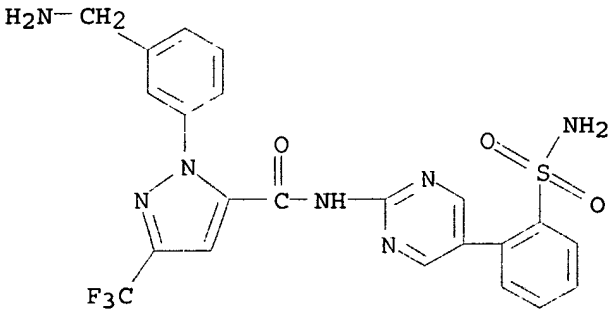
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-40-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

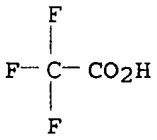
CM 1

CRN 209957-39-1
CMF C22 H18 F3 N7 O3 S

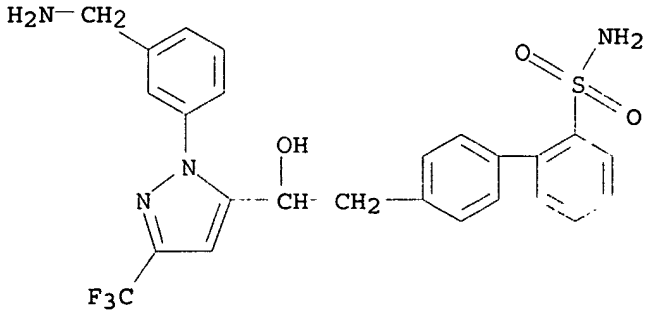


CM 2

CRN 76-05-1
CMF C2 H F3 O2



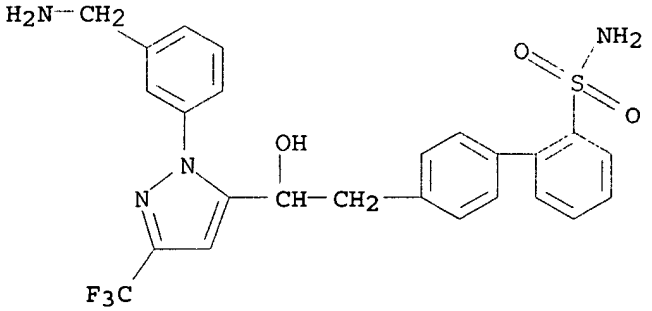
RN 209957-45-9 CAPLUS
CN [1,1'-Biphenyl]-2-sulfonamide, 4'-[2-[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]-2-hydroxyethyl]- (9CI) (CA INDEX NAME)



RN 209957-46-0 CAPLUS
CN [1,1'-Biphenyl]-2-sulfonamide, 4'-[2-[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]-2-hydroxyethyl]-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

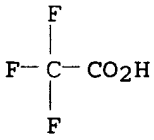
CM 1

CRN 209957-45-9
CMF C25 H23 F3 N4 O3 S

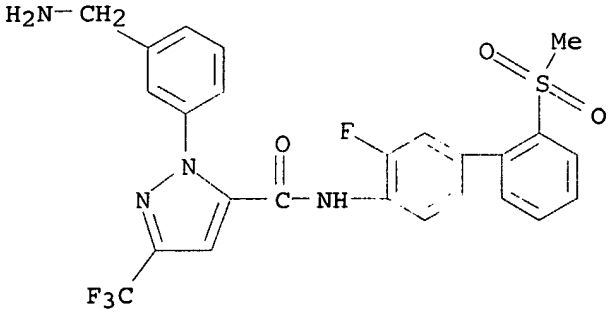


CM 2

CRN 76-05-1
CMF C2 H F3 O2



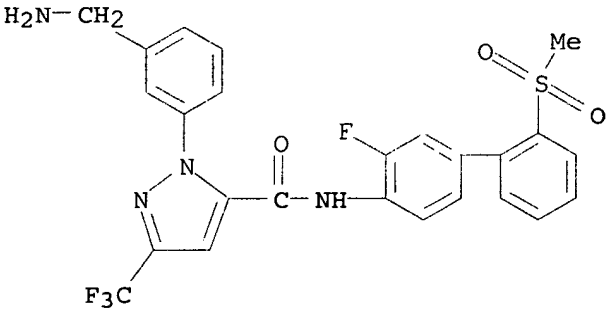
RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-48-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

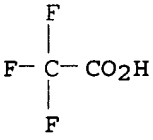
CM 1

CRN 209957-47-1
CMF C25 H20 F4 N4 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

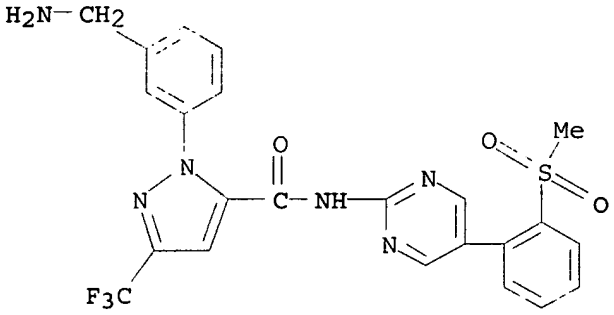


RN 209957-50-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

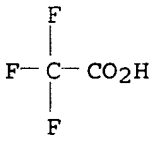
CRN 209957-49-3

CMF C23 H19 F3 N6 O3 S

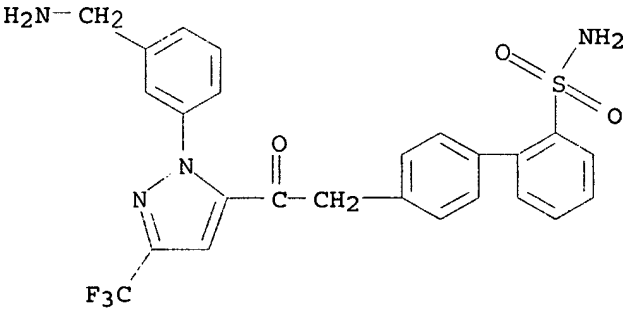


CM 2

CRN 76-05-1
CMF C2 H F3 O2



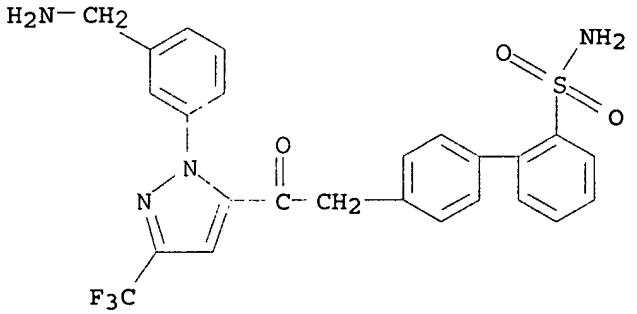
RN 209957-55-1 CAPLUS
CN [1,1'-Biphenyl]-2-sulfonamide, 4'-[2-[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]-2-oxoethyl]- (9CI) (CA INDEX NAME)



RN 209957-56-2 CAPLUS
CN [1,1'-Biphenyl]-2-sulfonamide, 4'-[2-[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]-2-oxoethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

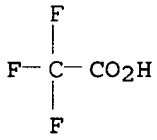
CM 1

CRN 209957-55-1
CMF C25 H21 F3 N4 O3 S

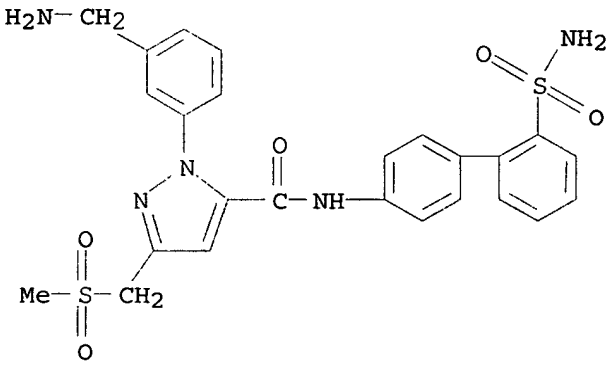


CM 2

CRN 76-05-1
CMF C2 H F3 O2



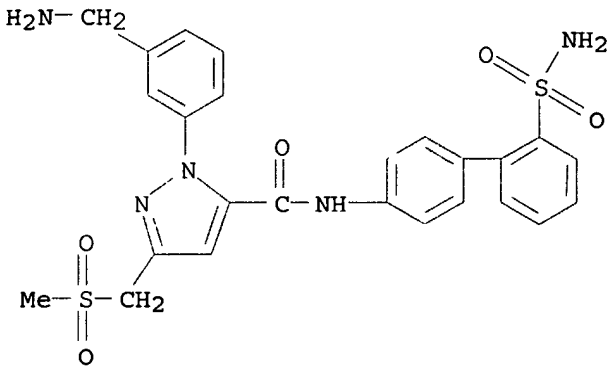
RN 209957-57-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-[(methylsulfonyl)methyl]- (9CI) (CA INDEX NAME)



RN 209957-58-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-[(methylsulfonyl)methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

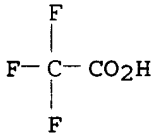
CM 1

CRN 209957-57-3
CMF C25 H25 N5 O5 S2

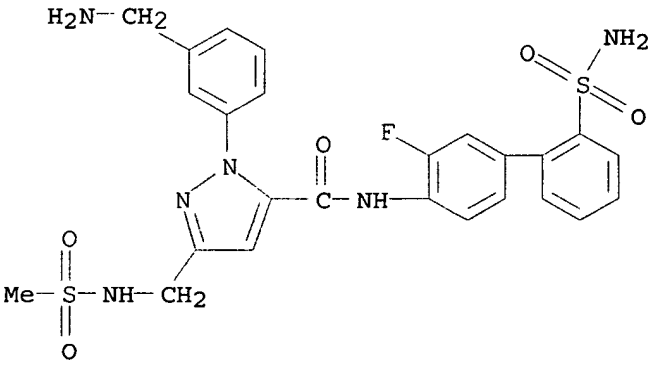


CM 2

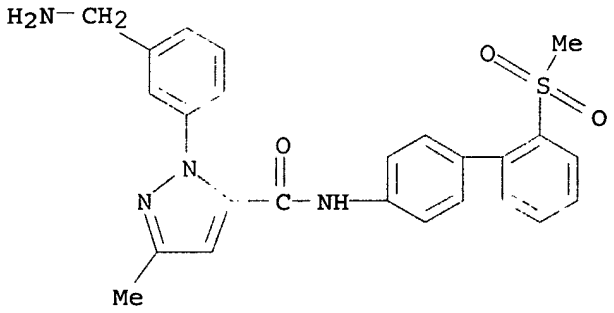
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-61-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-[[(methylsulfonyl)amino]methyl]- (9CI) (CA INDEX NAME)



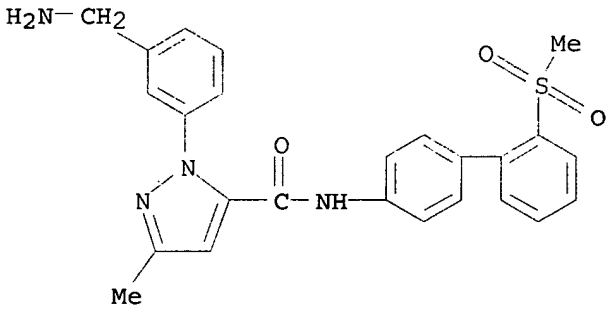
RN 209957-65-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-methyl-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 209957-66-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-methyl-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

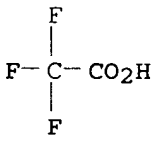
CM 1

CRN 209957-65-3
CMF C25 H24 N4 O3 S

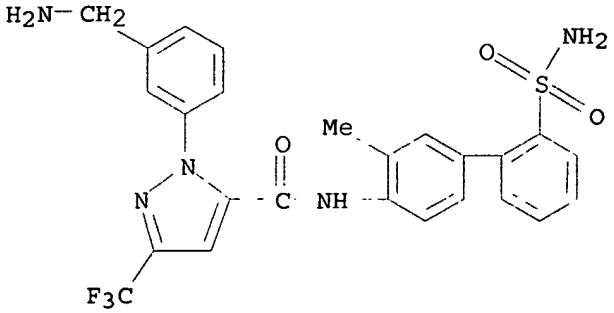


CM 2

CRN 76-05-1
CMF C2 H F3 O2



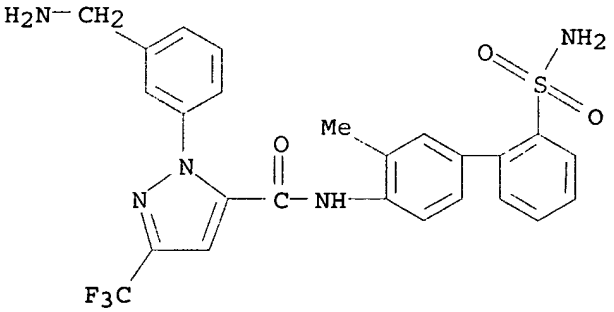
RN 209957-67-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-68-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

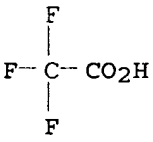
CM 1

CRN 209957-67-5
CMF C25 H22 F3 N5 O3 S

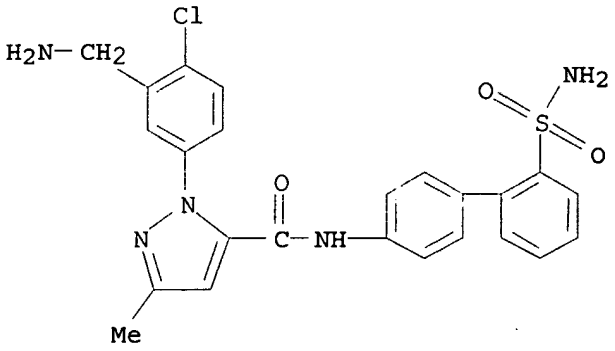


CM 2

CRN 76-05-1
CMF C2 H F3 O2



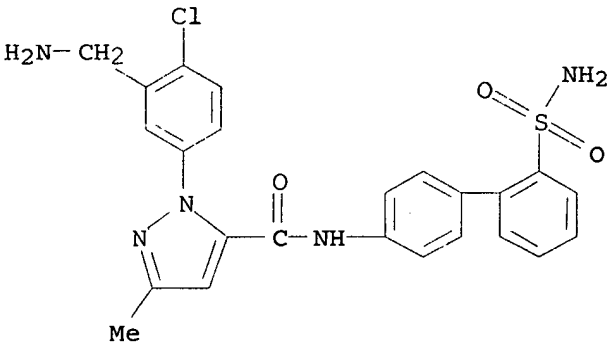
RN 209957-71-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-chlorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209957-72-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-chlorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

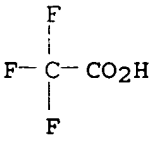
CM 1

CRN 209957-71-1
CMF C24 H22 Cl N5 O3 S

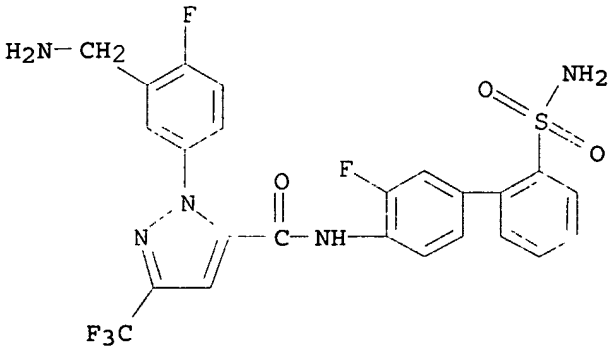


CM 2

CRN 76-05-1
CMF C2 H F3 O2



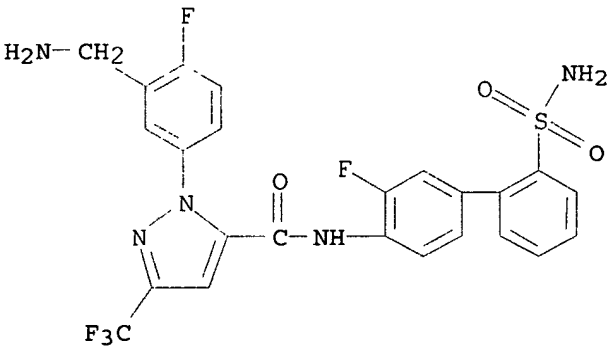
RN 209957-73-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-74-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

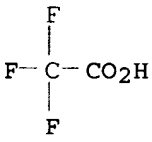
CM 1

CRN 209957-73-3
CMF C24 H18 F5 N5 O3 S

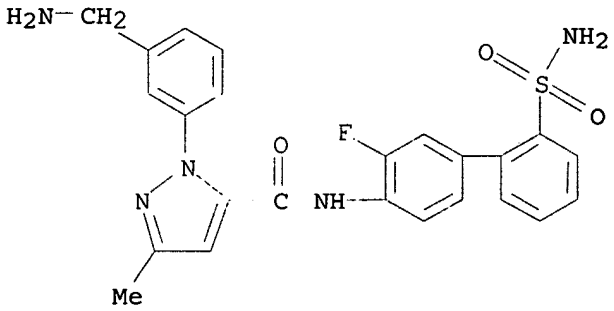


CM 2

CRN 76-05-1
CMF C2 H F3 O2



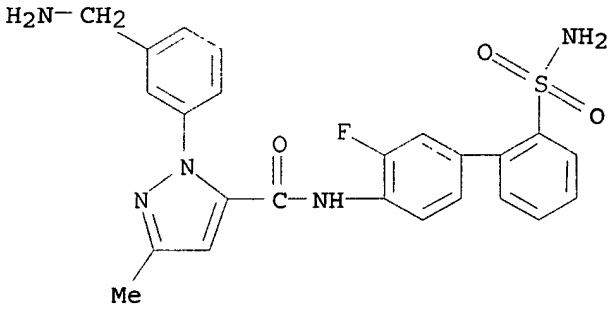
RN 209957-75-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209957-76-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

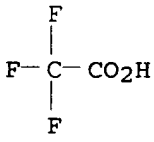
CM 1

CRN 209957-75-5
CMF C24 H22 F N5 O3 S

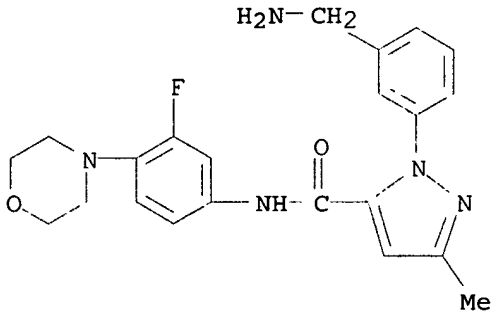


CM 2

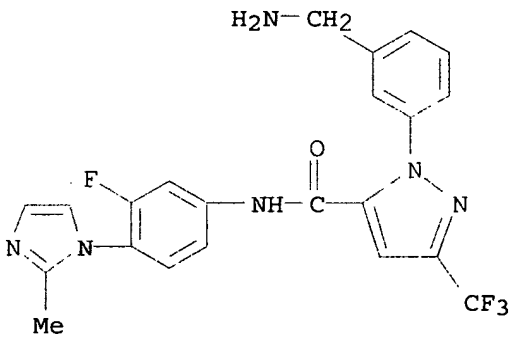
CRN 76-05-1
CMF C2 H F3 O2



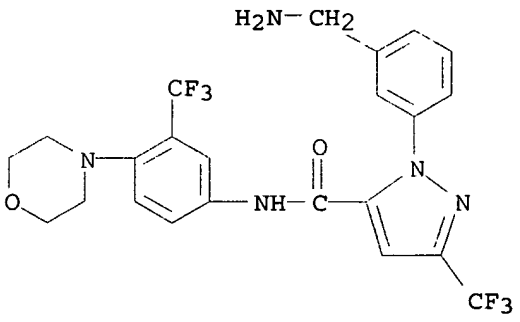
RN 209957-81-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(4-morpholinyl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209957-83-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-92-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

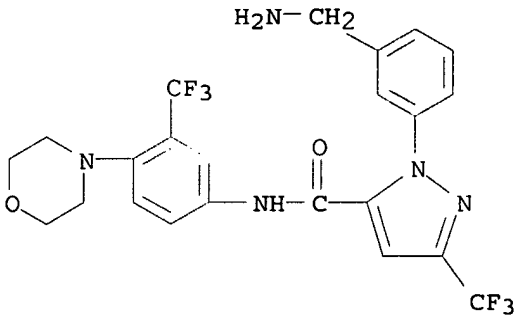


RN 209957-93-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

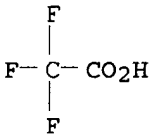
CRN 209957-92-6

CMF C23 H21 F6 N5 O2

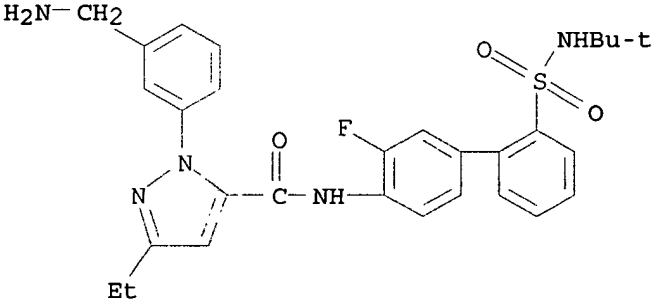


CM 2

CRN 76-05-1
CMF C2 H F3 O2



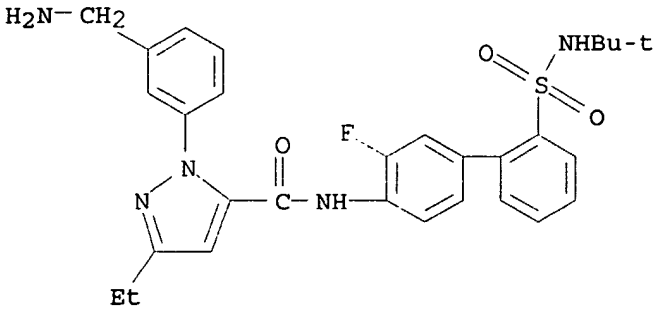
RN 209957-94-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-ethyl- (9CI) (CA INDEX NAME)



RN 209957-95-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-ethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

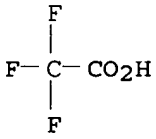
CM 1

CRN 209957-94-8
CMF C29 H32 F N5 O3 S

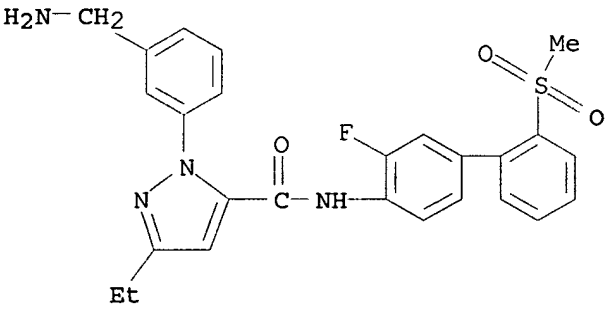


CM 2

CRN 76-05-1
CMF C2 H F3 O2



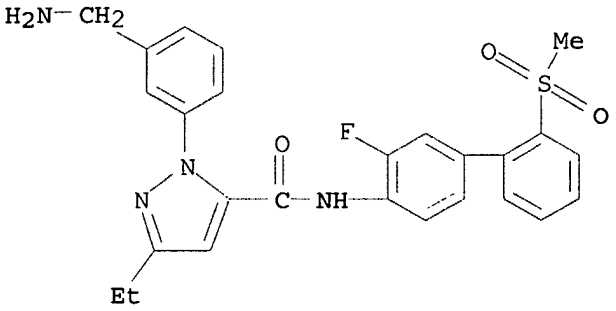
RN 209957-96-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-ethyl-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 209957-97-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-ethyl-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

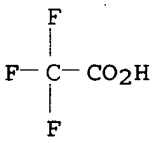
CM 1

CRN 209957-96-0
CMF C26 H25 F N4 O3 S

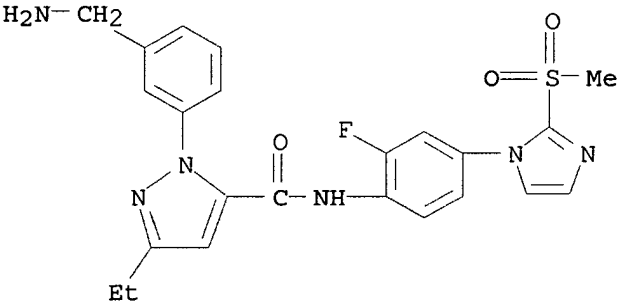


CM 2

CRN 76-05-1
CMF C2 H F3 O2



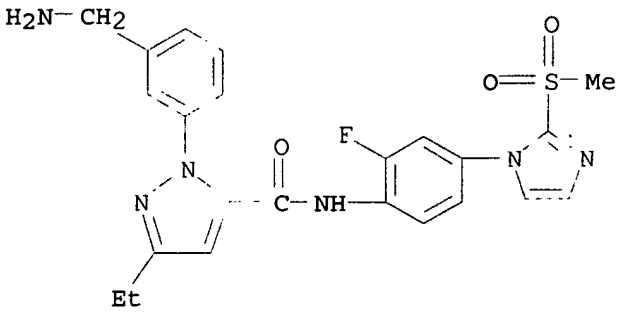
RN 209957-98-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-ethyl-N-[2-fluoro-4-[2-(methylsulfonyl)-1H-imidazol-1-yl]phenyl]- (9CI) (CA INDEX NAME)



RN 209957-99-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-ethyl-N-[2-fluoro-4-[2-(methylsulfonyl)-1H-imidazol-1-yl]phenyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

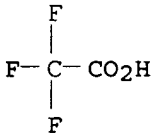
CM 1

CRN 209957-98-2
CMF C23 H23 F N6 O3 S

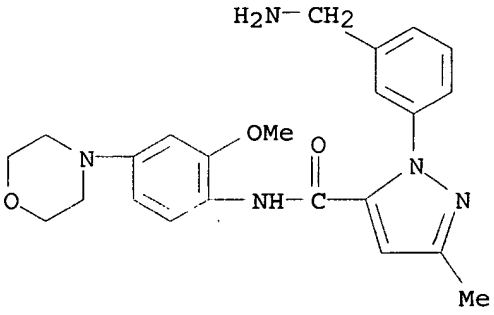


CM 2

CRN 76-05-1
CMF C2 H F3 O2



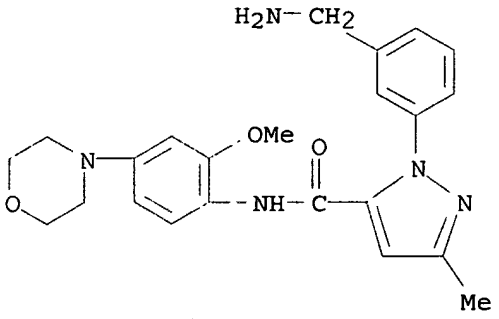
RN 209958-07-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-methoxy-4-(4-morpholinyl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209958-08-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-methoxy-4-(4-morpholinyl)phenyl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

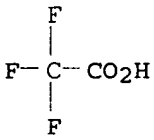
CM 1

CRN 209958-07-6
CMF C23 H27 N5 O3

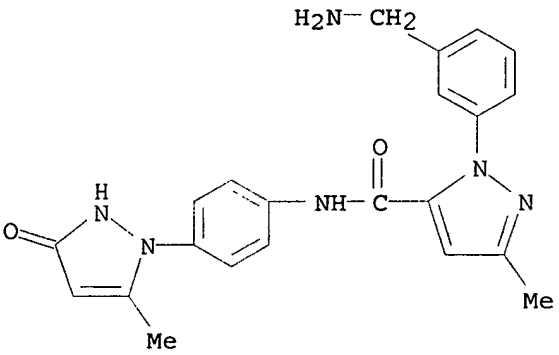


CM 2

CRN 76-05-1
CMF C2 H F3 O2



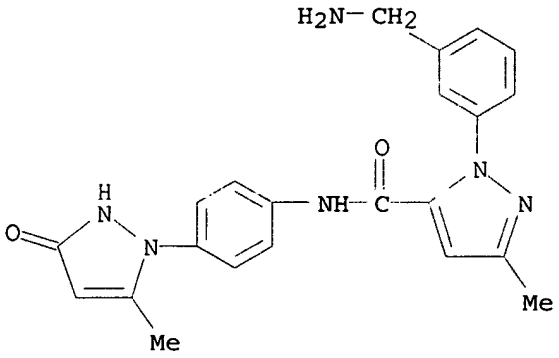
RN 209958-09-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209958-10-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

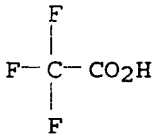
CM 1

CRN 209958-09-8
CMF C22 H22 N6 O2

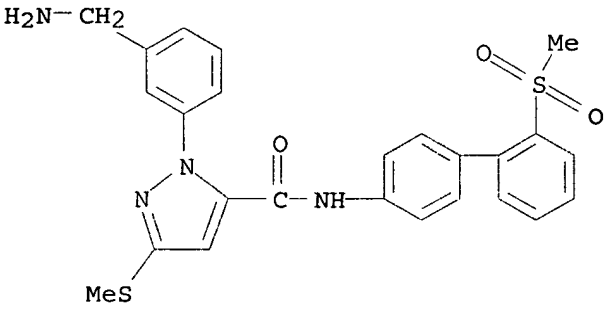


CM 2

CRN 76-05-1
CMF C2 H F3 O2



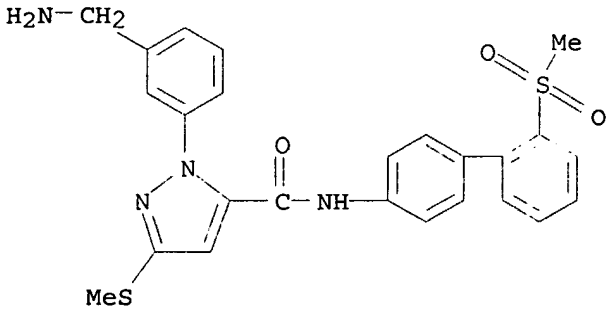
RN 209958-11-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylthio)- (9CI) (CA INDEX NAME)



RN 209958-12-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylthio)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

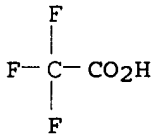
CM 1

CRN 209958-11-2
CMF C25 H24 N4 O3 S2

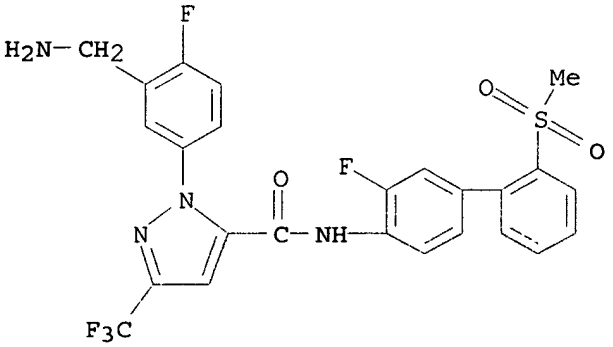


CM 2

CRN 76-05-1
CMF C2 H F3 O2



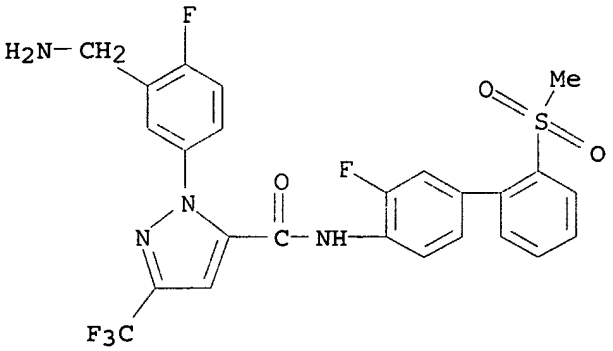
RN 209958-13-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209958-14-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

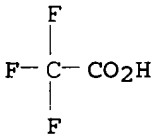
CM 1

CRN 209958-13-4
CMF C25 H19 F5 N4 O3 S

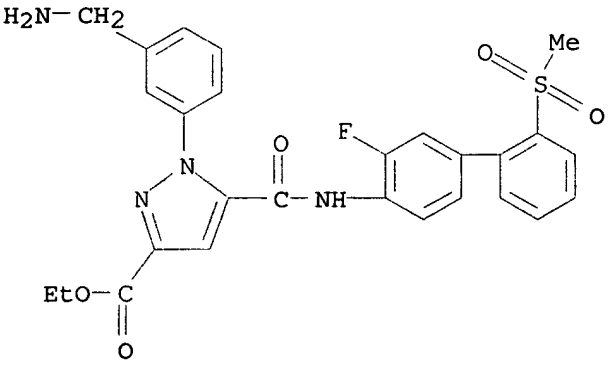


CM 2

CRN 76-05-1
CMF C2 H F3 O2



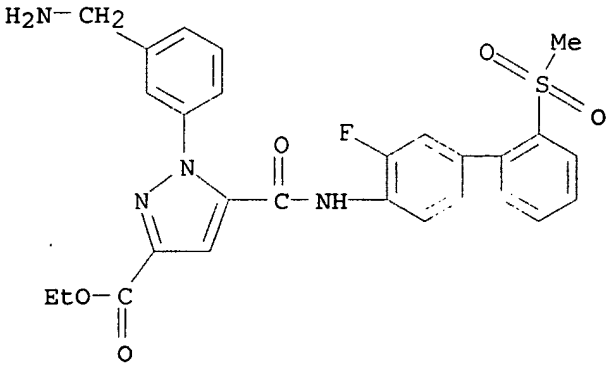
RN 209958-15-6 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 209958-16-7 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

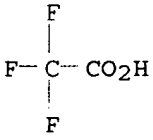
CM 1

CRN 209958-15-6
CMF C27 H25 F N4 O5 S

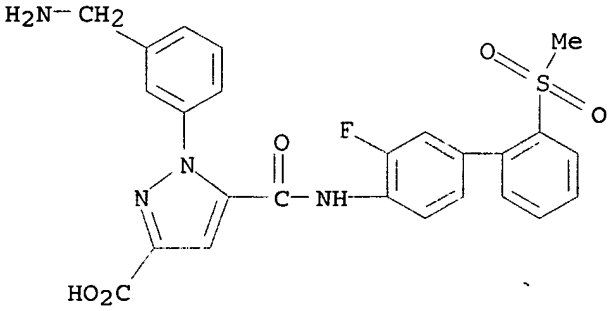


CM 2

CRN 76-05-1
CMF C2 H F3 O2



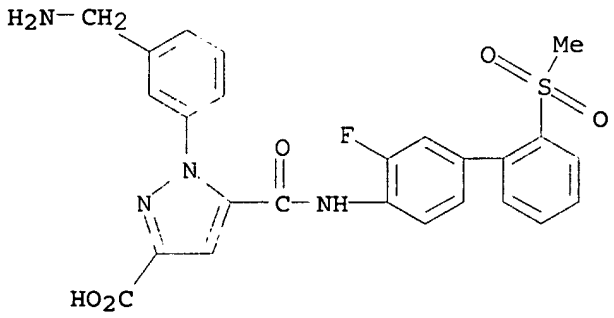
RN 209958-17-8 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)



RN 209958-18-9 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

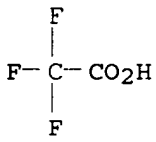
CM 1

CRN 209958-17-8
CMF C25 H21 F N4 O5 S

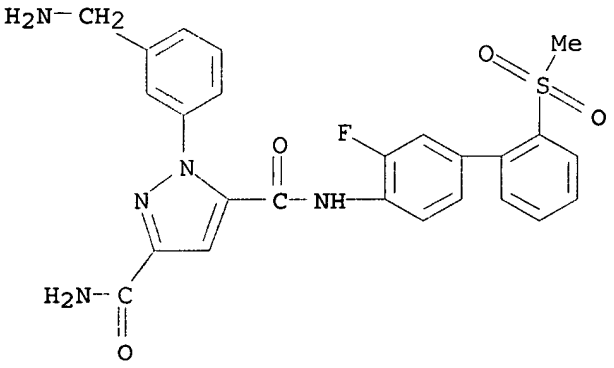


CM 2

CRN 76-05-1
CMF C2 H F3 O2



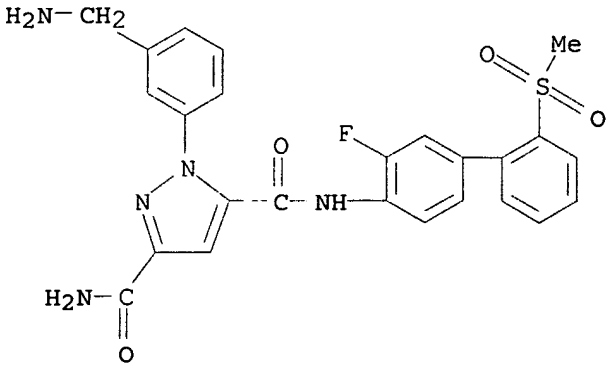
RN 209958-19-0 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxamide, 1-[3-(aminomethyl)phenyl]-N5-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 209958-20-3 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxamide, 1-[3-(aminomethyl)phenyl]-N5-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

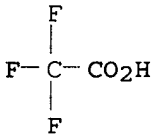
CM 1

CRN 209958-19-0
CMF C25 H22 F N5 O4 S

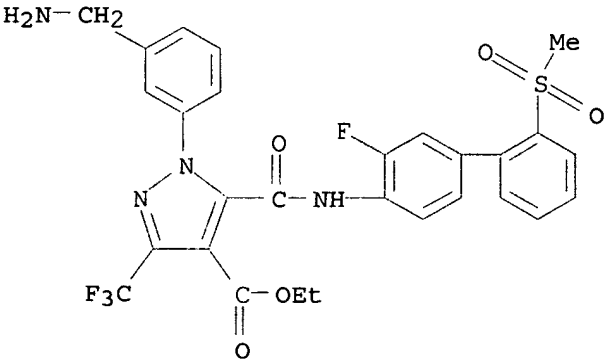


CM 2

CRN 76-05-1
CMF C2 H F3 O2



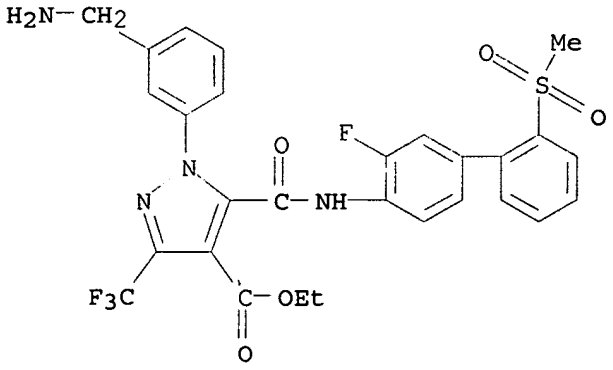
RN 209958-21-4 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 209958-22-5 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

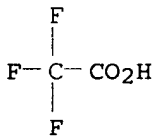
CM 1

CRN 209958-21-4
CMF C28 H24 F4 N4 O5 S

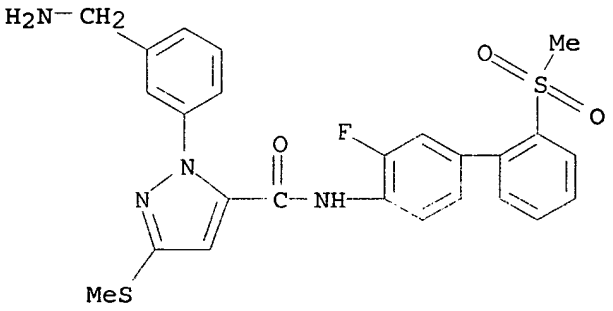


CM 2

CRN 76-05-1
CMF C2 H F3 O2



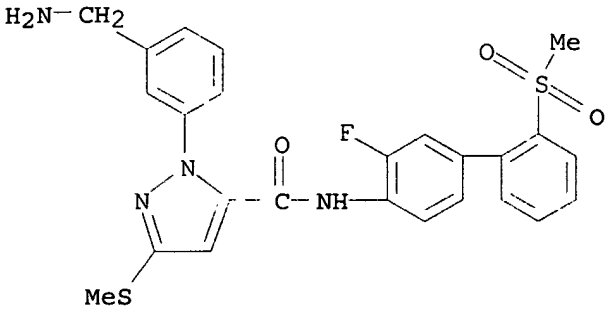
RN 209958-24-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylthio)- (9CI) (CA INDEX NAME)



RN 209958-25-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylthio)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

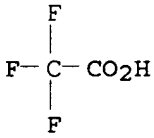
CM 1

CRN 209958-24-7
CMF C25 H23 F N4 O3 S2

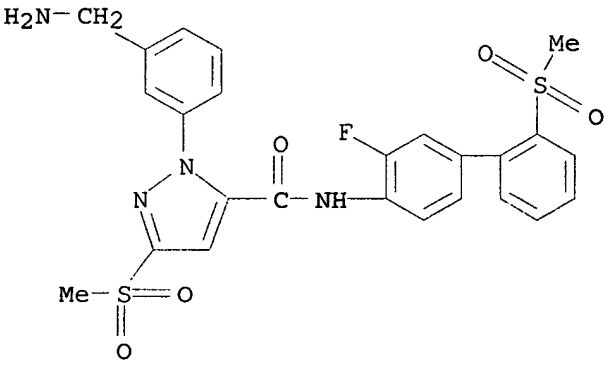


CM 2

CRN 76-05-1
CMF C2 H F3 O2



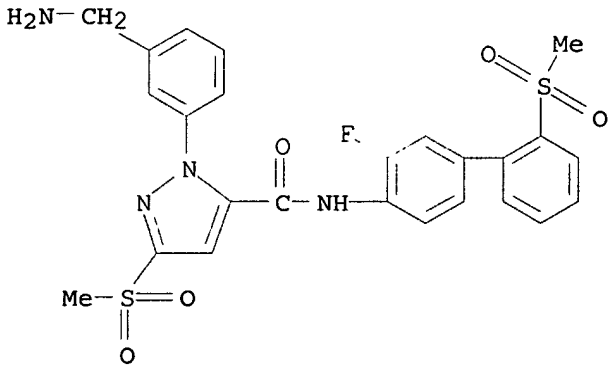
RN 209958-26-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylsulfonyl)- (9CI) (CA INDEX NAME)



RN 209958-27-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylsulfonyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

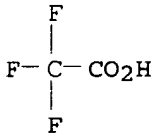
CM 1

CRN 209958-26-9
CMF C25 H23 F N4 O5 S2

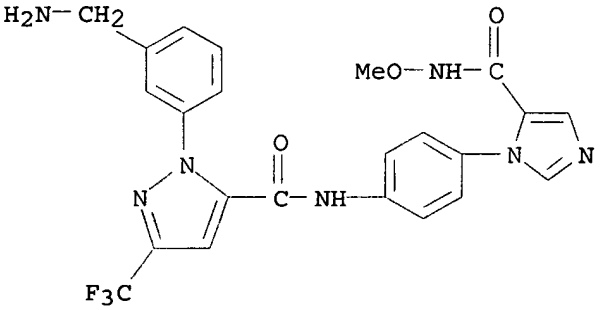


CM 2

CRN 76-05-1
CMF C2 H F3 O2



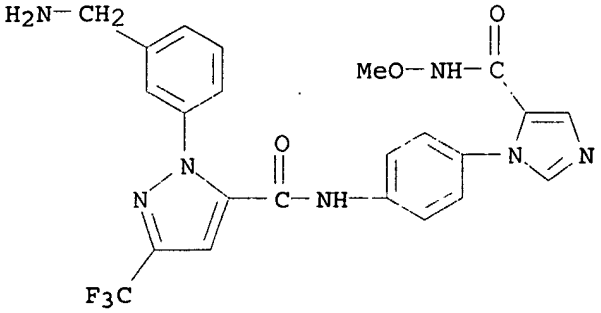
RN 209958-28-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-[(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209958-29-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-[(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

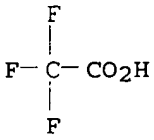
CM 1

CRN 209958-28-1
CMF C23 H20 F3 N7 O3

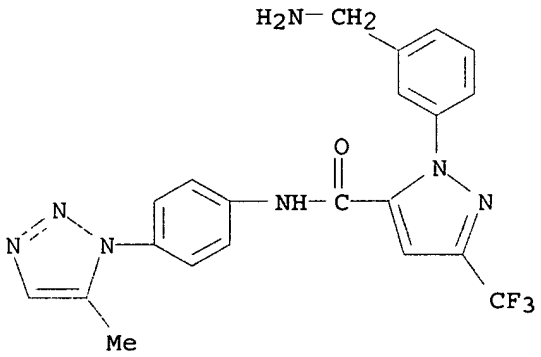


CM 2

CRN 76-05-1
CMF C2 H F3 O2



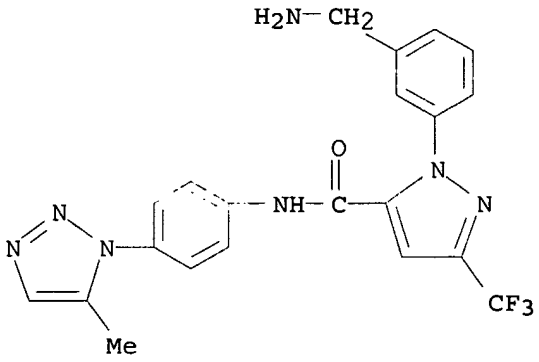
RN 209958-30-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209958-31-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

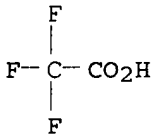
CM 1

CRN 209958-30-5
CMF C21 H18 F3 N7 O



CM 2

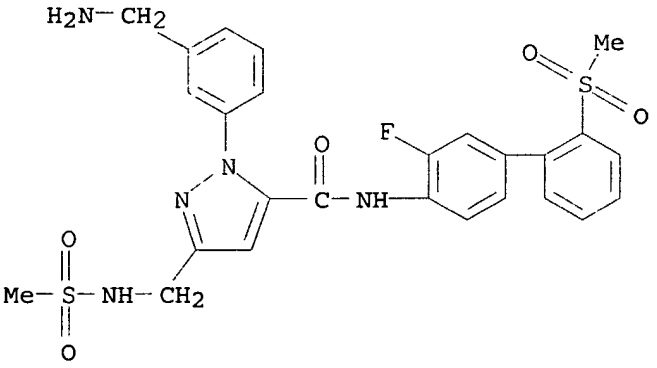
CRN 76-05-1
CMF C2 H F3 O2



RN 256512-27-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-[[(methylsulfonyl)amino]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

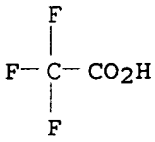
CRN 256512-26-2
CMF C26 H26 F N5 O5 S2



CM 2

CRN 76-05-1

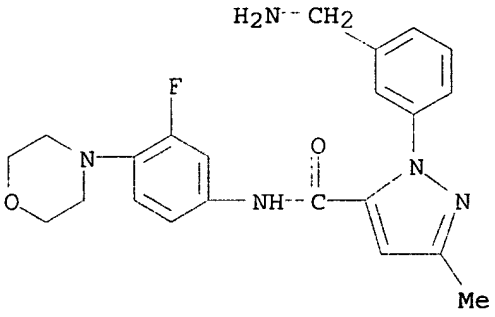
CMF C2 H F3 O2



RN 256512-29-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(4-morpholinyl)phenyl]-3-methyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

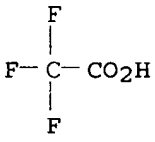
CM 1

CRN 209957-81-3
CMF C22 H24 F N5 O2



CM 2

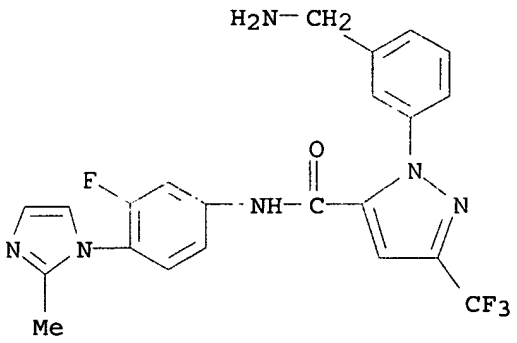
CRN 76-05-1
CMF C2 H F3 O2



RN 256512-30-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

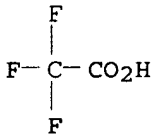
CM 1

CRN 209957-83-5
CMF C22 H18 F4 N6 O

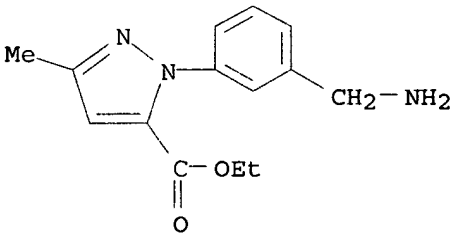


CM 2

CRN 76-05-1
CMF C2 H F3 O2

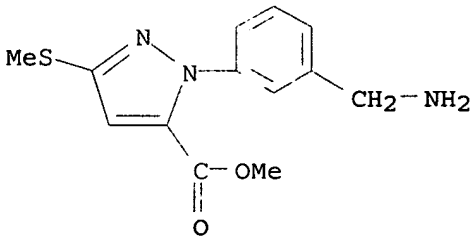


IT **209960-83-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of azoles as Factor Xa inhibitors)
RN 209960-83-8 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-[3-(aminomethyl)phenyl]-3-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT **209960-51-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azoles as Factor Xa inhibitors)
RN 209960-51-0 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-[3-(aminomethyl)phenyl]-3-(methylthio)-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

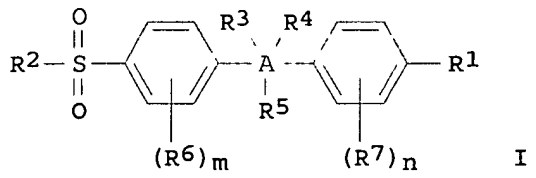
L7 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:795808 CAPLUS
DOCUMENT NUMBER: 132:35714
TITLE: Preparation of heterocyclyl sulfonylbenzene compounds as anti-inflammatory/analgesic agents.
INVENTOR(S): Ando, Kazuo; Kato, Tomoki; Kawai, Akiyoshi; Nonomura, Tomomi
PATENT ASSIGNEE(S): Pfizer Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 236 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9964415	A1	19991216	WO 1999-IB970		19990531
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
AU 9938414	A1	19991230	AU 1999-38414		19990531
EP 1086097	A1	20010328	EP 1999-921043		19990531
EP 1086097	B1	20040519			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI					
JP 2002517496	T2	20020618	JP 2000-553424		19990531
AT 267196	E	20040615	AT 1999-921043		19990531
PT 1086097	T	20040831	PT 1999-921043		19990531
ES 2220060	T3	20041201	ES 1999-921043		19990531
ZA 9903897	A	20010104	ZA 1999-3897		19990610
US 6294558	B1	20010925	US 1999-446049		19991215
US 2002045654	A1	20020418	US 2001-841348		20010424
US 6608095	B2	20030819			
US 2003225064	A1	20031204	US 2003-465767		20030618
US 6727238	B2	20040427			
US 2004157824	A1	20040812	US 2004-771861		20040203
US 6949536	B2	20050927			
PRIORITY APPLN. INFO.:			WO 1998-IB912	W	19980611
			WO 1999-IB970	W	19990531
			US 1999-446049	A3	19991215

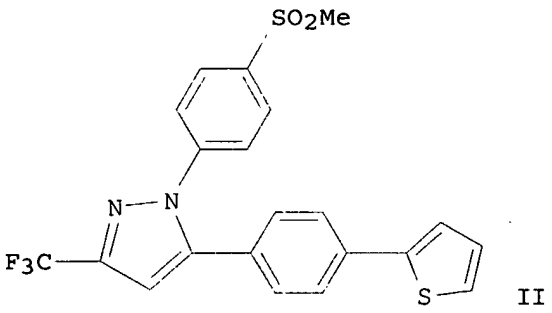
US 2001-841348 A3 20010424
US 2003-465767 A3 20030618

OTHER SOURCE(S): MARPAT 132:35714

GI



I



II

AB This invention provides a compound of formula (I) or its pharmaceutically acceptable salt thereof [wherein A is partially unsatd. or unsatd. five membered heterocyclic, or partially unsatd. or unsatd. five membered carbocyclic, wherein the 4-(sulfonyl)phenyl and the 4-substituted Ph in formula I are attached to ring atoms of Ring A, which are adjacent to each other; R1 is optionally substituted aryl or heteroaryl, with the proviso that when A is pyrazole, R1 is heteroaryl; R2 is C1-4 alkyl, halo-substituted C1-4 alkyl, C1-4 alkylamino, C1-4 dialkylamino or amino; R3, R4 and R5 are independently hydrogen, halo, C1-4 alkyl, halo-substituted C1-4 alkyl or the like; or two of R3, R4 and R5 are taken together with atoms to which they are attached and form a 4-7 membered ring; R6 and R7 are independently hydrogen, halo, C1-4 alkyl, halo-substituted C1-4 alkyl, C1-4 alkoxy, C1-4 alkylthio, C1-4 alkylamino or N,N-di C1-4 alkylamino; and m and n are independently 1, 2, 3 or 4]. This invention also provides a pharmaceutical composition useful for the treatment of a medical condition in which prostaglandins are implicated as pathogens. This invention relates to compound and pharmaceutical compns. for the treatment of cyclooxygenase mediated diseases. These compds. inhibit the biosynthesis of prostaglandins by intervention of the action of the enzyme cyclooxygenase on arachidonic acid, and are therefore useful in the treatment or alleviation of inflammation and other inflammation associated disorders, such as arthritis, in mammals (no data). Thus, To a stirred solution of 1-[4-(Methylsulfonyl)phenyl]-5-(4-bromophenyl)-3-trifluoromethyl-1H-pyrazole (0.27 g) in DME (8 mL) was added 3-thiophenboronic acid (0.09 g), bis(triphenylphosphine)palladium(II)chloride (0.05 g) and saturated NaHCO3 solution (2 mL) at room temperature under nitrogen.

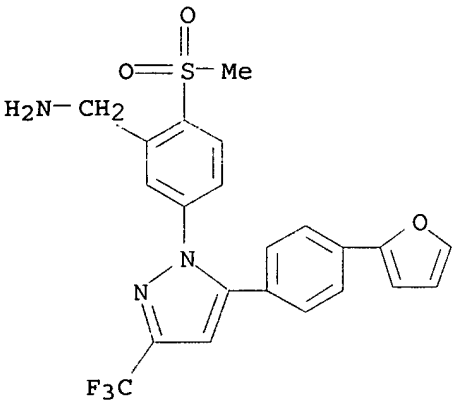
The mixture was heated at reflux temperature for 16 h, and cooled down to room temperature to give, after purification by flash chromatog. eluting with Et acetate/hexane (1/1), 1-[4-(Methylsulfonyl)phenyl]-5-[4-(2-thienyl)phenyl]-3-trifluoromethyl-1H-pyrazole (II) in 64 % yield.

IT **252560-57-9P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclyl sulfonylbenzene compds. as cyclooxygenase inhibitors, prostaglandin biosynthesis inhibitors, anti-inflammatory, and analgesic agents)

RN 252560-57-9 CAPLUS

CN Benzenemethanamine, 5-[5-[4-(2-furanyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]-2-(methylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 35 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:479506 CAPLUS

DOCUMENT NUMBER: 129:109090

TITLE: Preparation of nitrogen-containing heteroaromatics as factor Xa inhibitors

INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell; Cacciola, Joseph; Fevig, John Matthew; Han, Qi; Orwat, Michael James; Quan, Mimi Lifen; Rossi, Karen Anita

PATENT ASSIGNEE(S): The Dupont Merck Pharmaceutical Co., USA

SOURCE: PCT Int. Appl., 438 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

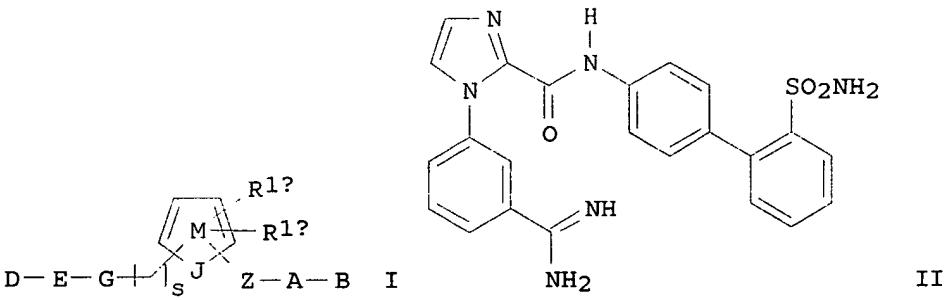
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9828269	A1	19980702	WO 1997-US22895	19971215
W: AM, AU, AZ, BR, BY, CA, CN, CZ, EE, HU, IL, JP, KG, KR, KZ, LT, LV, MD, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2275796	AA	19980702	CA 1997-2275796	19971215

AU 9856020	A1	19980717	AU 1998-56020		19971215
AU 730224	B2	20010301			
EP 946508	A1	19991006	EP 1997-952409		19971215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI					
EE 9900316	A	20000215	EE 1999-316		19971215
SI 20017	C	20000229	SI 1997-20082		19971215
CN 1246847	A	20000308	CN 1997-181852		19971215
BR 9714073	A	20000509	BR 1997-14073		19971215
JP 2001509145	T2	20010710	JP 1998-528845		19971215
ZA 9711586	A	19990701	ZA 1997-11586		19971223
TW 492971	B	20020701	TW 1997-86119637		19980203
NO 9902633	A	19990820	NO 1999-2633		19990601
NO 313190	B1	20020826			
MX 9905878	A	20000131	MX 1999-5878		19990622
LT 4673	B	20000725	LT 1999-76		19990622
LV 12430	B	20000720	LV 1999-99		19990730
PRIORITY APPLN. INFO.:			US 1996-769859	A	19961223
			US 1997-879944	A	19970620
			WO 1997-US22895	W	19971215

OTHER SOURCE(S): MARPAT 129:109090

GI



AB The title compds. [I; ring M contains, in addition to J, 0-3 N atoms; J = N, NH; D = CN, C(:NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G = absent, NHCH2, OCH2, etc.; Z = C1-4 alkylene, (CH2)rO(CH2)r, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, C1-6 alkyl, etc.; R8, R9 = H, C1-6 alkyl, (CH2)nPh; n = 0-3; r = 0-3; s = 0-2], useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-[o-(tert-BuSO2)phenyl]aniline with Me3Al/hexane in CH2Cl2 followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the Pinner reaction of the resulting intermediate afforded the title compound II. A number of compds. I were found to exhibit a Ki of ≤ 10 μM against factor Xa. Some compds. I were evaluated and found to exhibit Ki of < 10 μM against thrombin.

IT **209958-16-7P**

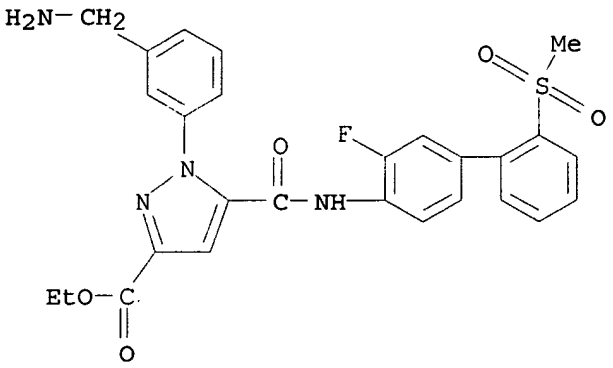
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors)

RN 209958-16-7 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

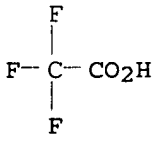
CM 1

CRN 209958-15-6
CMF C27 H25 F N4 O5 S



CM 2

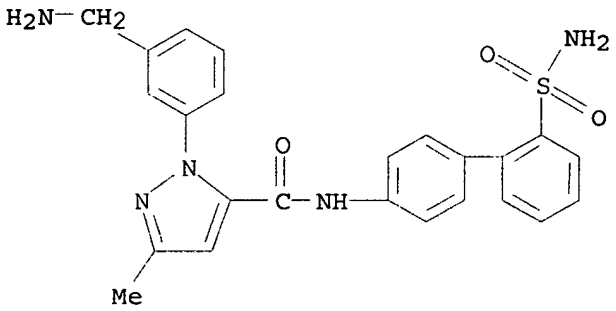
CRN 76-05-1
CMF C2 H F3 O2



IT 209955-58-8P 209955-59-9P 209955-60-2P
209955-61-3P 209956-42-3P 209956-93-4P
209956-94-5P 209956-95-6P 209956-96-7P
209956-97-8P 209956-98-9P 209956-99-0P
209957-00-6P 209957-27-7P 209957-28-8P
209957-29-9P 209957-30-2P 209957-31-3P
209957-32-4P 209957-33-5P 209957-34-6P
209957-35-7P 209957-36-8P 209957-37-9P
209957-38-0P 209957-39-1P 209957-40-4P
209957-45-9P 209957-46-0P 209957-47-1P
209957-48-2P 209957-49-3P 209957-50-6P
209957-55-1P 209957-56-2P 209957-57-3P
209957-58-4P 209957-61-9P 209957-62-0P
209957-65-3P 209957-66-4P 209957-67-5P
209957-68-6P 209957-71-1P 209957-72-2P
209957-73-3P 209957-74-4P 209957-75-5P
209957-76-6P 209957-77-7P 209957-78-8P
209957-81-3P 209957-82-4P 209957-83-5P
209957-84-6P 209957-92-6P 209957-93-7P
209957-94-8P 209957-95-9P 209957-96-0P

209957-97-1P 209957-98-2P 209957-99-3P
209958-07-6P 209958-08-7P 209958-09-8P
209958-10-1P 209958-11-2P 209958-12-3P
209958-13-4P 209958-14-5P 209958-15-6P
209958-17-8P 209958-18-9P 209958-19-0P
209958-20-3P 209958-21-4P 209958-22-5P
209958-24-7P 209958-25-8P 209958-26-9P
209958-27-0P 209958-28-1P 209958-29-2P
209958-30-5P 209958-31-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors)

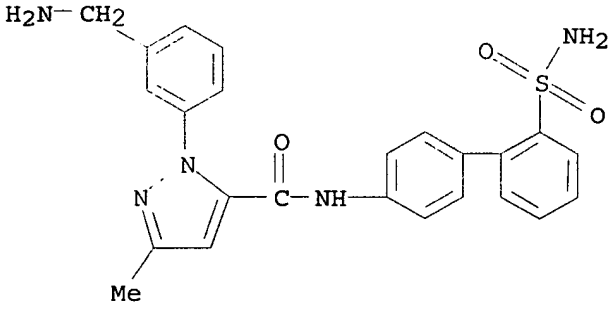
RN 209955-58-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209955-59-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

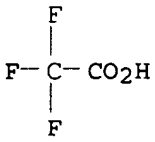
CM 1

CRN 209955-58-8
CMF C24 H23 N5 O3 S

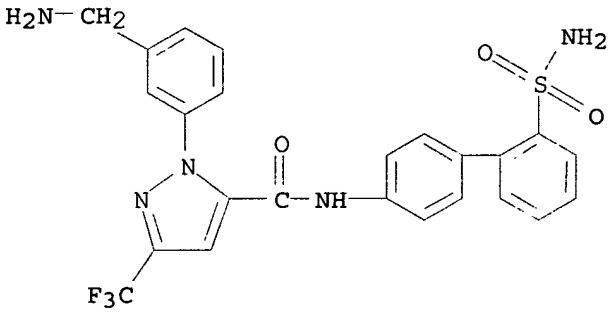


CM 2

CRN 76-05-1
CMF C2 H F3 O2



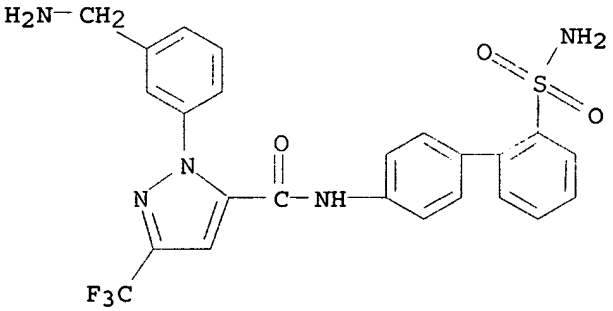
RN 209955-60-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-61-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

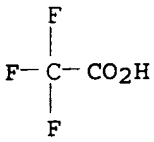
CM 1

CRN 209955-60-2
CMF C24 H20 F3 N5 O3 S

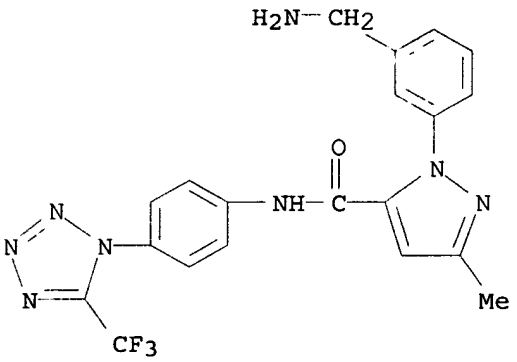


CM 2

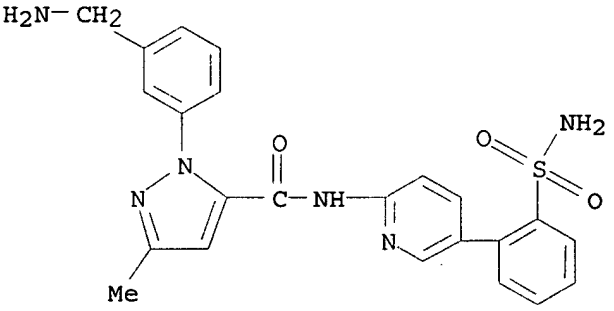
CRN 76-05-1
CMF C2 H F3 O2



RN 209956-42-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-methyl-N-[4-[5-(trifluoromethyl)-1H-tetrazol-1-yl]phenyl]- (9CI) (CA INDEX NAME)



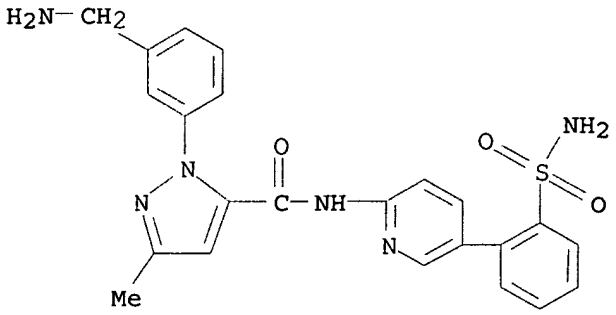
RN 209956-93-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209956-94-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

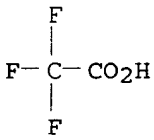
CM 1

CRN 209956-93-4
CMF C23 H22 N6 O3 S

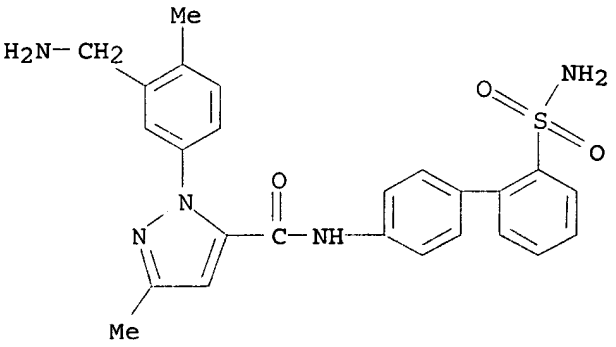


CM 2

CRN 76-05-1
CMF C2 H F3 O2



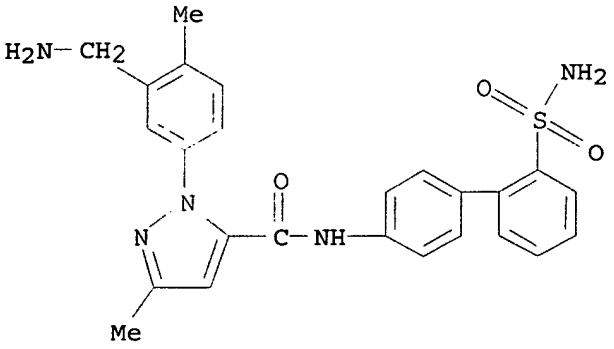
RN 209956-95-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-methylphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209956-96-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-methylphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

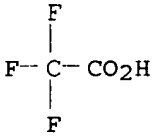
CM 1

CRN 209956-95-6
CMF C25 H25 N5 O3 S

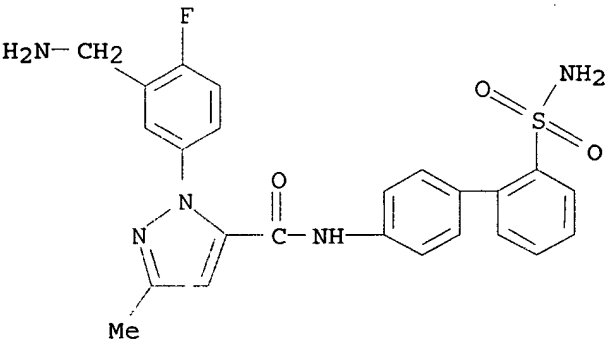


CM 2

CRN 76-05-1
CMF C2 H F3 O2



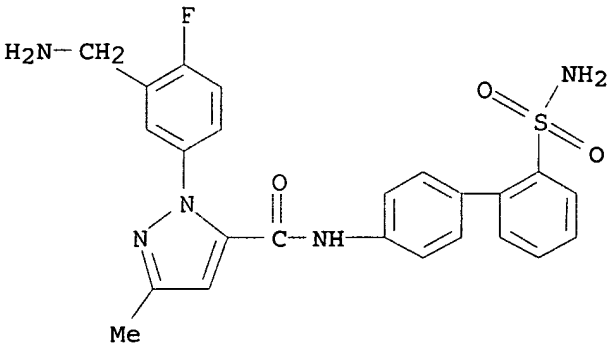
RN 209956-97-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209956-98-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

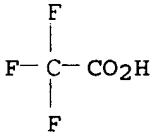
CM 1

CRN 209956-97-8
CMF C24 H22 F N5 O3 S

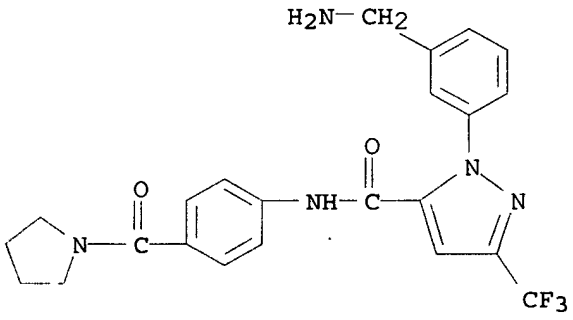


CM 2

CRN 76-05-1
CMF C2 H F3 O2



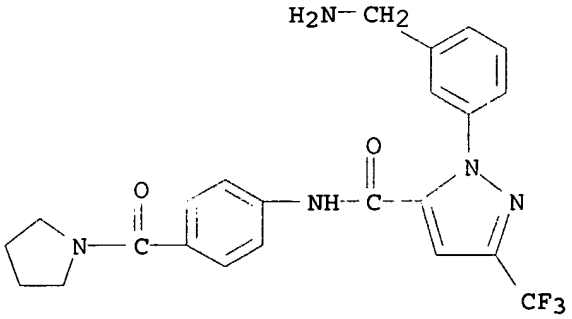
RN 209956-99-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-00-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

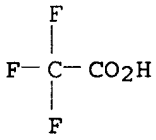
CM 1

CRN 209956-99-0
CMF C23 H22 F3 N5 O2

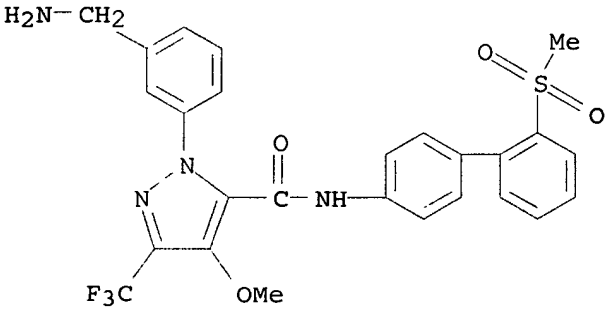


CM 2

CRN 76-05-1
CMF C2 H F3 O2



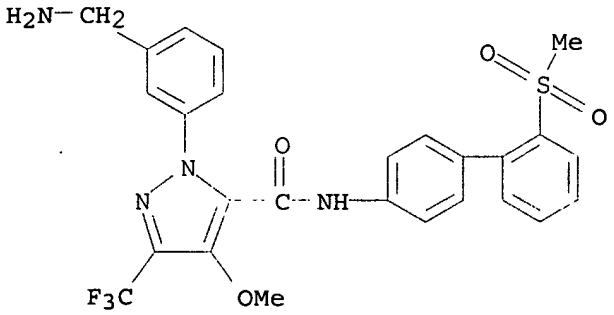
RN 209957-27-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-28-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

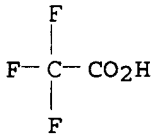
CM 1

CRN 209957-27-7
CMF C26 H23 F3 N4 O4 S

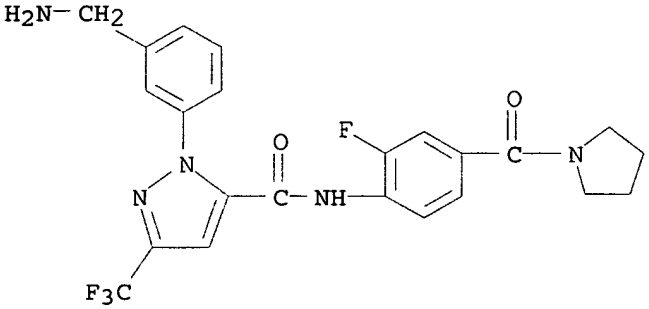


CM 2

CRN 76-05-1
CMF C2 H F3 O2



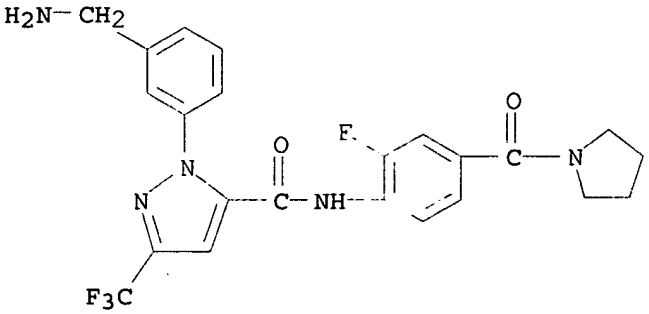
RN 209957-29-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-30-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

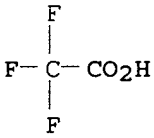
CM 1

CRN 209957-29-9
CMF C23 H21 F4 N5 O2

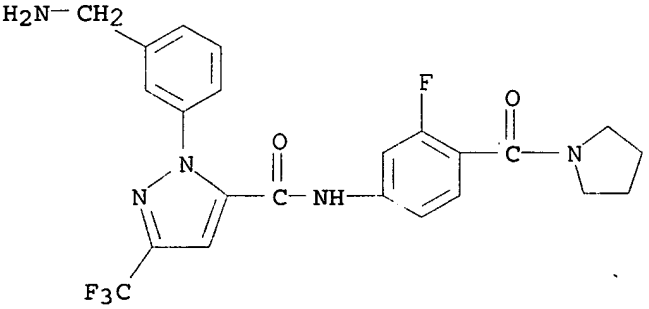


CM 2

CRN 76-05-1
CMF C2 H F3 O2



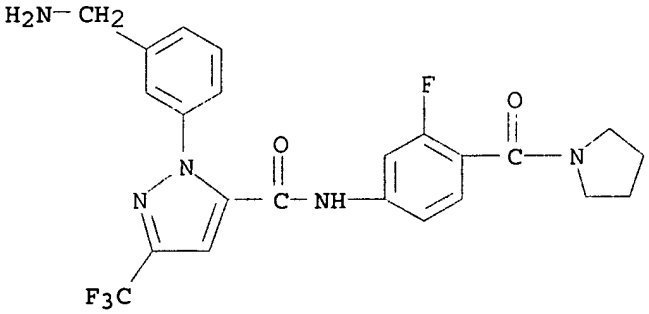
RN 209957-31-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-32-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

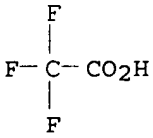
CM 1

CRN 209957-31-3
CMF C23 H21 F4 N5 O2

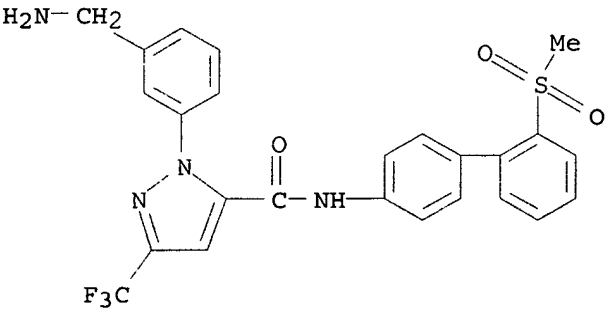


CM 2

CRN 76-05-1
CMF C2 H F3 O2



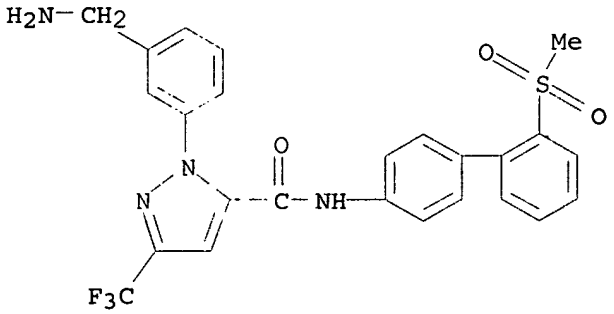
RN 209957-33-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-34-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

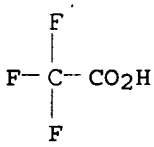
CM 1

CRN 209957-33-5
CMF C25 H21 F3 N4 O3 S

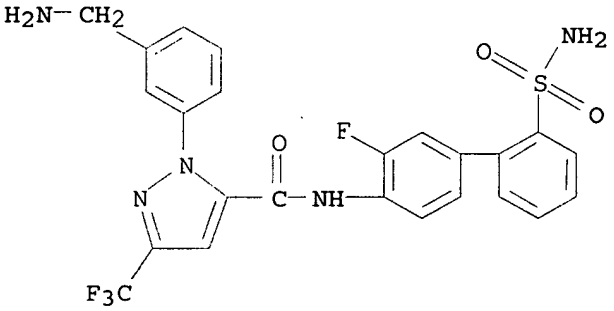


CM 2

CRN 76-05-1
CMF C2 H F3 O2



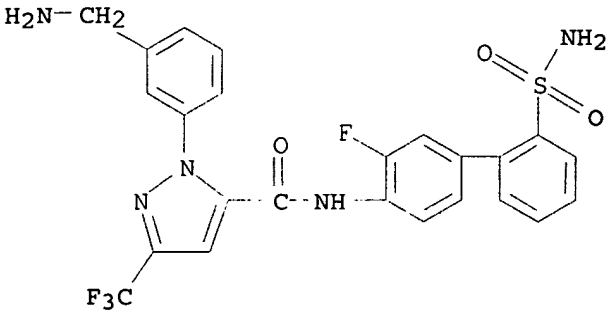
RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-36-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

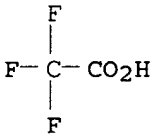
CM 1

CRN 209957-35-7
CMF C24 H19 F4 N5 O3 S

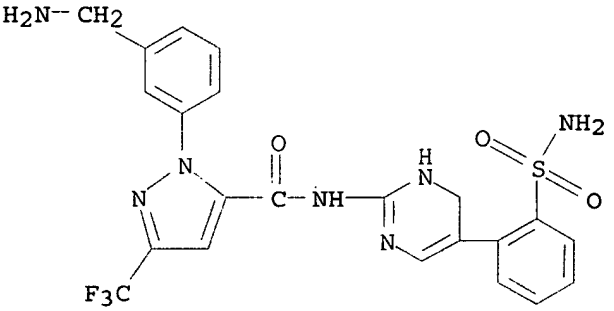


CM 2

CRN 76-05-1
CMF C2 H F3 O2



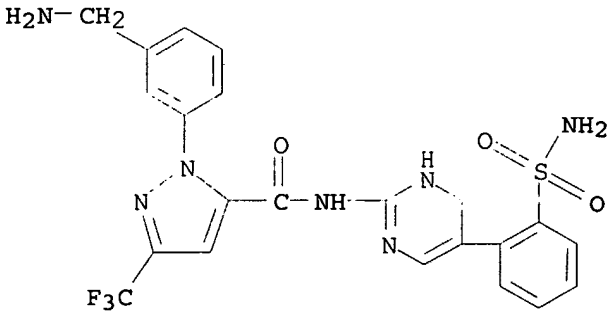
RN 209957-37-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-1,4-dihydro-2-pyrimidinyl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)



RN 209957-38-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-1,4-dihydro-2-pyrimidinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

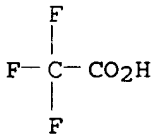
CM 1

CRN 209957-37-9
CMF C22 H20 F3 N7 O3 S

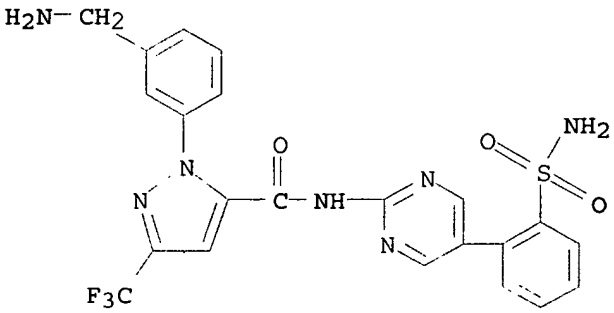


CM 2

CRN 76-05-1
CMF C2 H F3 O2



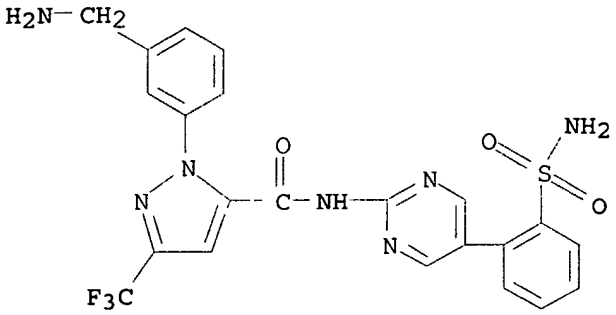
RN 209957-39-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-40-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

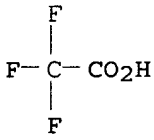
CM 1

CRN 209957-39-1
CMF C22 H18 F3 N7 O3 S

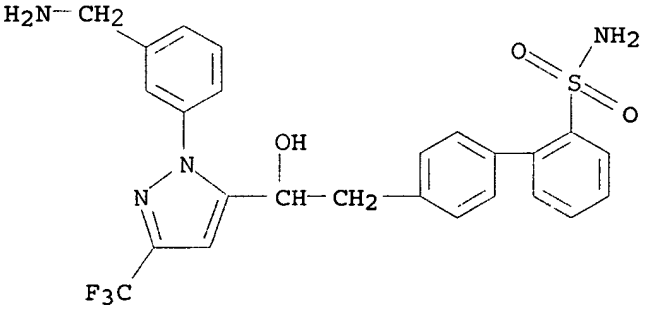


CM 2

CRN 76-05-1
CMF C2 H F3 O2



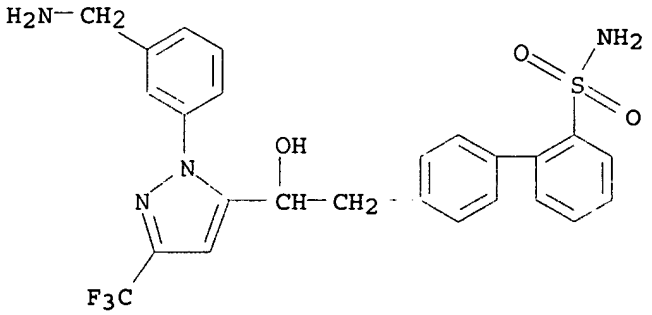
RN 209957-45-9 CAPLUS
CN [1,1'-Biphenyl]-2-sulfonamide, 4'-[2-[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]-2-hydroxyethyl]- (9CI) (CA INDEX NAME)



RN 209957-46-0 CAPLUS
CN [1,1'-Biphenyl]-2-sulfonamide, 4'-[2-[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]-2-hydroxyethyl]-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

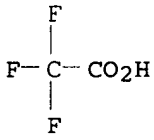
CM 1

CRN 209957-45-9
CMF C25 H23 F3 N4 O3 S

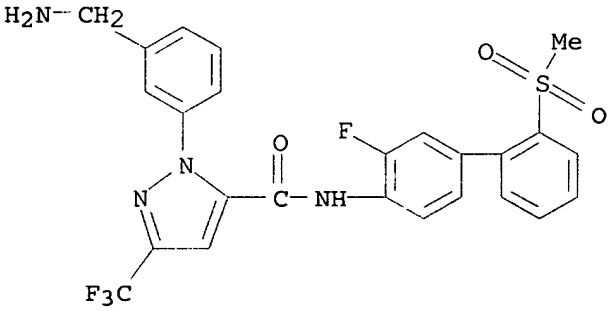


CM 2

CRN 76-05-1
CMF C2 H F3 O2



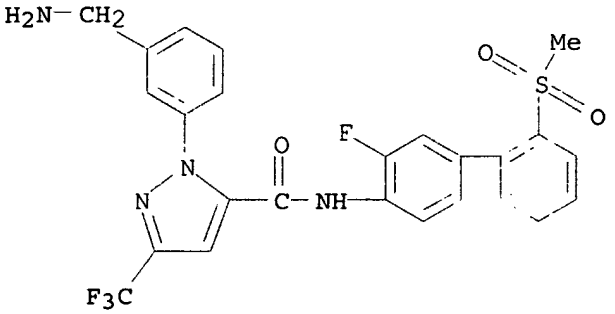
RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-48-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

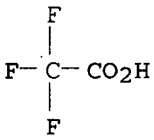
CM 1

CRN 209957-47-1
CMF C25 H20 F4 N4 O3 S

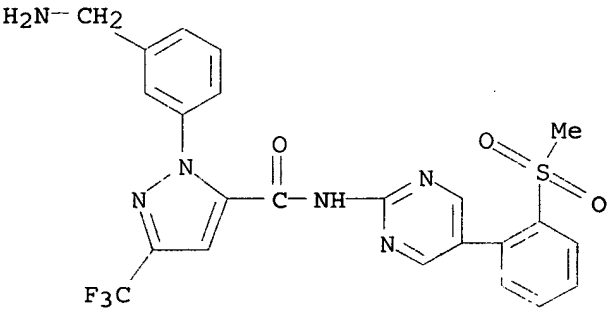


CM 2

CRN 76-05-1
CMF C2 H F3 O2



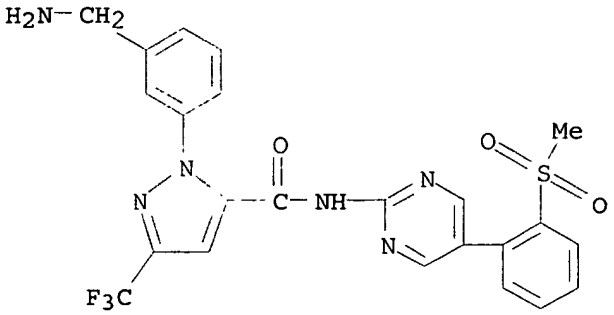
RN 209957-49-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-50-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

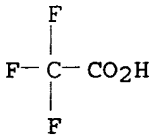
CM 1

CRN 209957-49-3
CMF C23 H19 F3 N6 O3 S

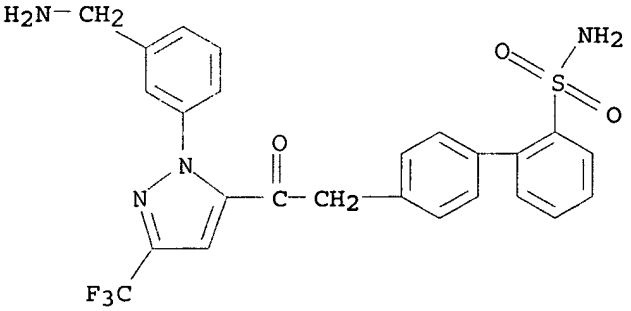


CM 2

CRN 76-05-1
CMF C2 H F3 O2



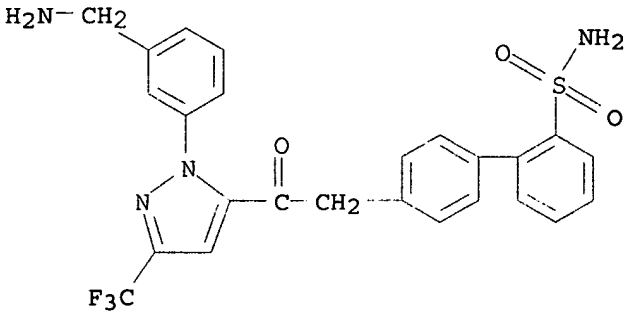
RN 209957-55-1 CAPLUS
CN [1,1'-Biphenyl]-2-sulfonamide, 4'-[2-[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]-2-oxoethyl]- (9CI) (CA INDEX NAME)



RN 209957-56-2 CAPLUS
CN [1,1'-Biphenyl]-2-sulfonamide, 4'-[2-[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]-2-oxoethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

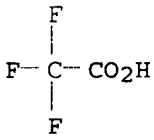
CM 1

CRN 209957-55-1
CMF C25 H21 F3 N4 O3 S

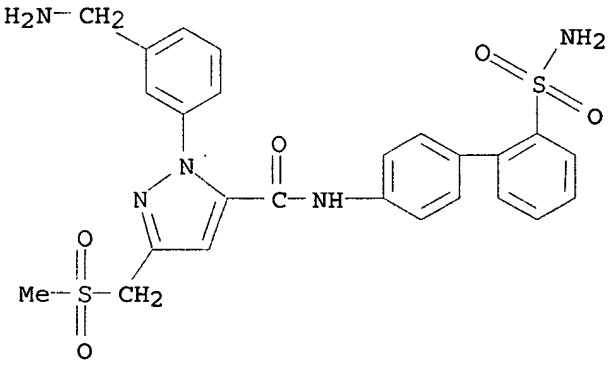


CM 2

CRN 76-05-1
CMF C2 H F3 O2



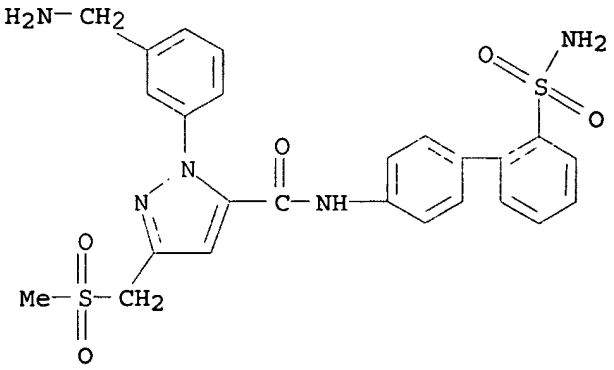
RN 209957-57-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-[(methylsulfonyl)methyl]- (9CI) (CA INDEX NAME)



RN 209957-58-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-[(methylsulfonyl)methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

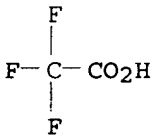
CM 1

CRN 209957-57-3
CMF C25 H25 N5 O5 S2

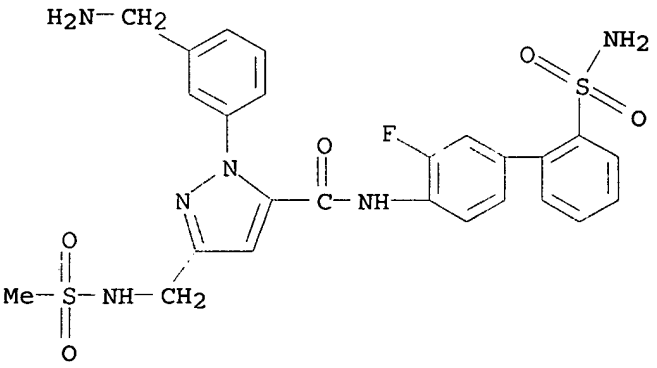


CM 2

CRN 76-05-1
CMF C2 H F3 O2



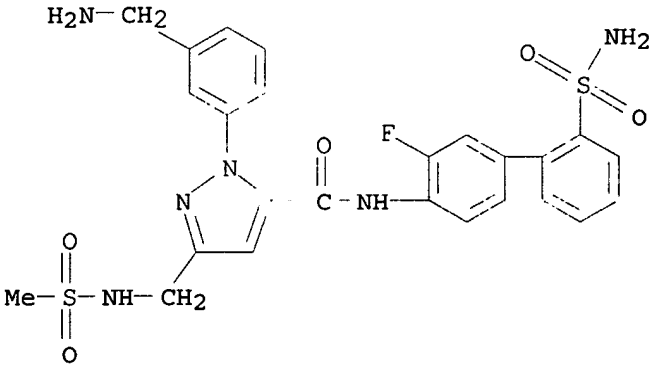
RN 209957-61-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-[[(methylsulfonyl)amino]methyl]- (9CI) (CA INDEX NAME)



RN 209957-62-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-[[(methylsulfonyl)amino]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

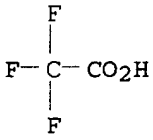
CM 1

CRN 209957-61-9
CMF C25 H25 F N6 O5 S2

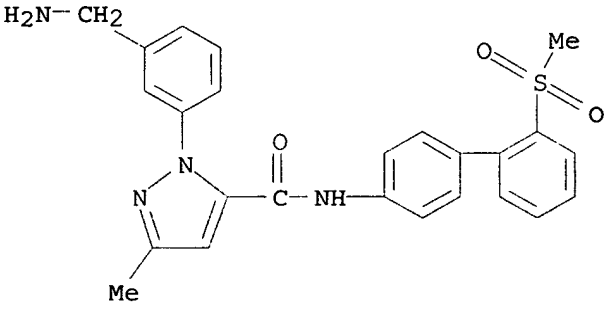


CM 2

CRN 76-05-1
CMF C2 H F3 O2



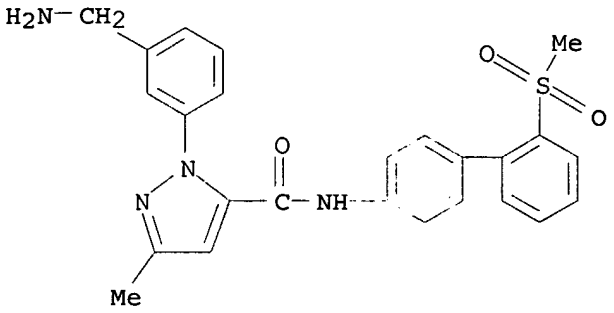
RN 209957-65-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-methyl-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 209957-66-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-methyl-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

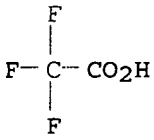
CM 1

CRN 209957-65-3
CMF C25 H24 N4 O3 S

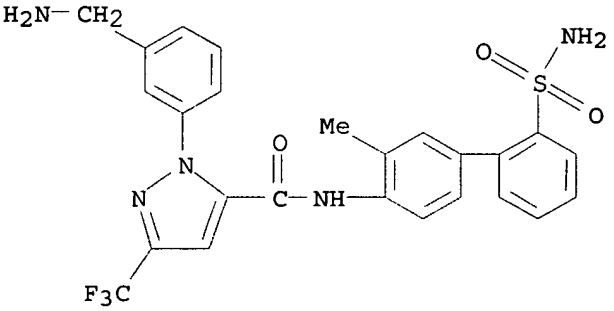


CM 2

CRN 76-05-1
CMF C2 H F3 O2



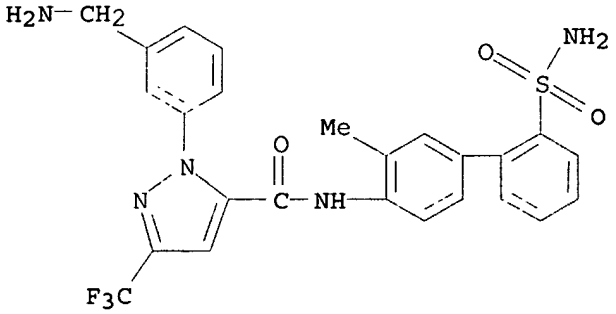
RN 209957-67-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-68-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

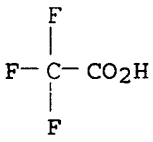
CM 1

CRN 209957-67-5
CMF C25 H22 F3 N5 O3 S

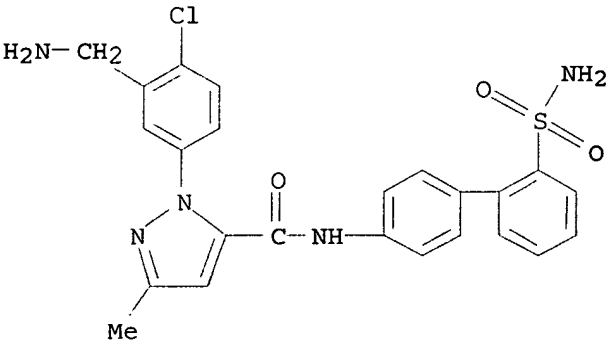


CM 2

CRN 76-05-1
CMF C2 H F3 O2



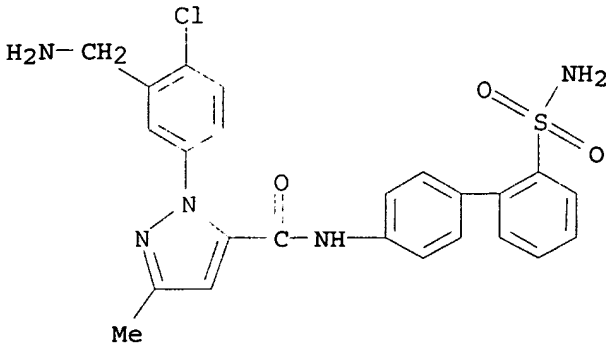
RN 209957-71-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-chlorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209957-72-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-chlorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

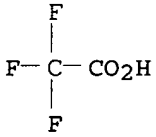
CM 1

CRN 209957-71-1
CMF C24 H22 Cl N5 O3 S

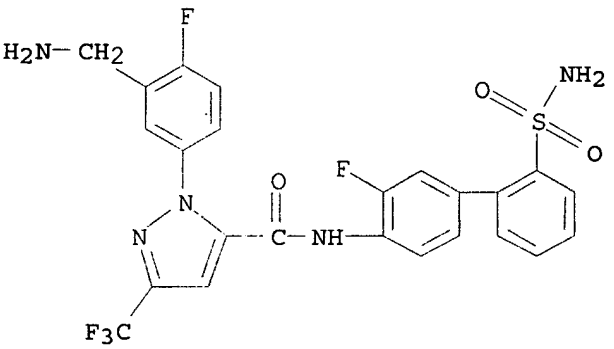


CM 2

CRN 76-05-1
CMF C2 H F3 O2



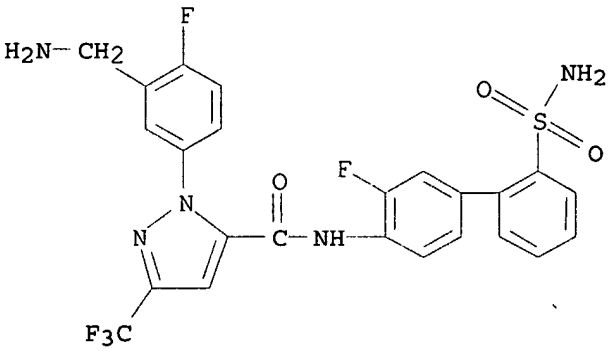
RN 209957-73-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-74-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

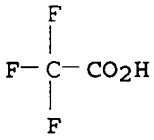
CM 1

CRN 209957-73-3
CMF C24 H18 F5 N5 O3 S

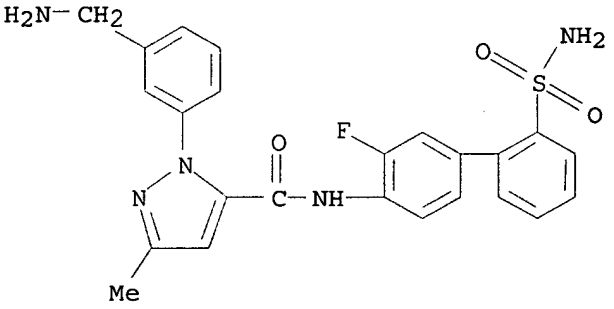


CM 2

CRN 76-05-1
CMF C2 H F3 O2



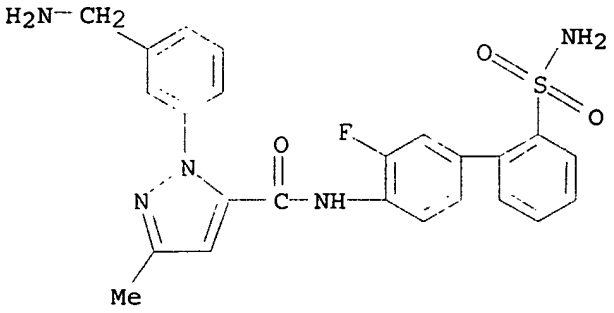
RN 209957-75-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209957-76-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

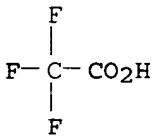
CM 1

CRN 209957-75-5
CMF C24 H22 F N5 O3 S

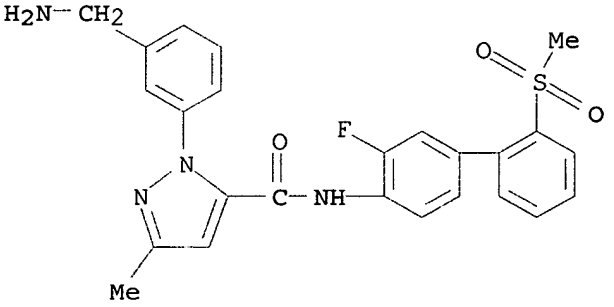


CM 2

CRN 76-05-1
CMF C2 H F3 O2



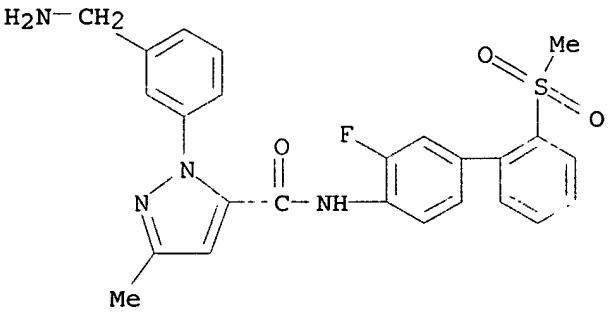
RN 209957-77-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209957-78-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

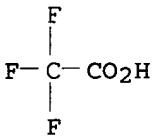
CM 1

CRN 209957-77-7
CMF C25 H23 F N4 O3 S

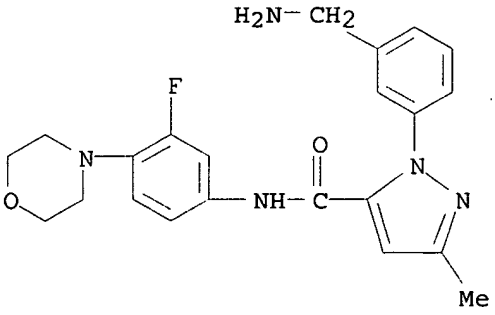


CM 2

CRN 76-05-1
CMF C2 H F3 O2



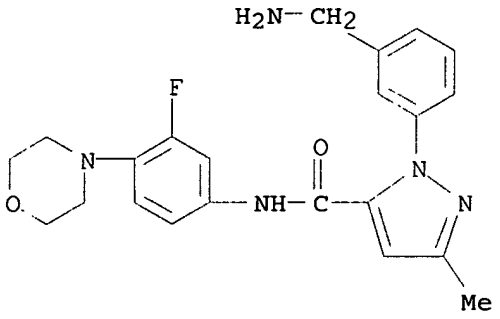
RN 209957-81-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(4-morpholinyl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209957-82-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(4-morpholinyl)phenyl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

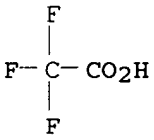
CM 1

CRN 209957-81-3
CMF C22 H24 F N5 O2

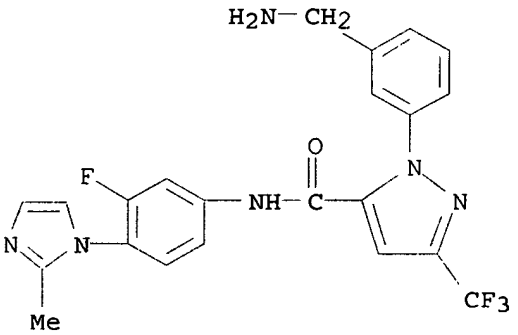


CM 2

CRN 76-05-1
CMF C2 H F3 O2



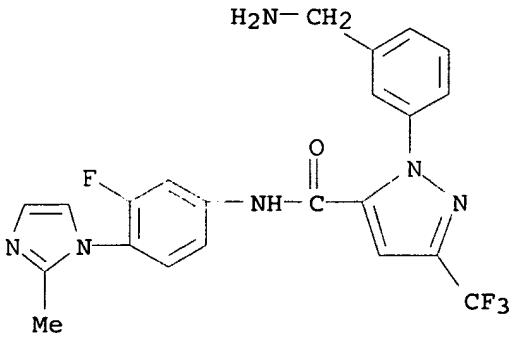
RN 209957-83-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-84-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

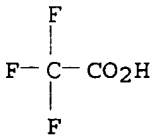
CM 1

CRN 209957-83-5
CMF C22 H18 F4 N6 O

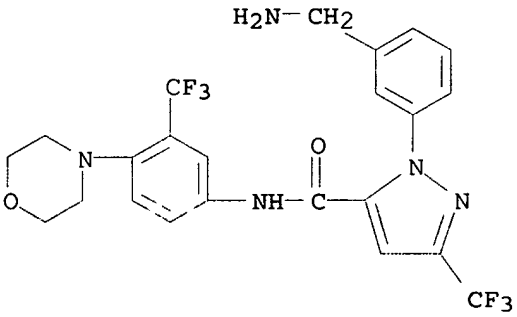


CM 2

CRN 76-05-1
CMF C2 H F3 O2



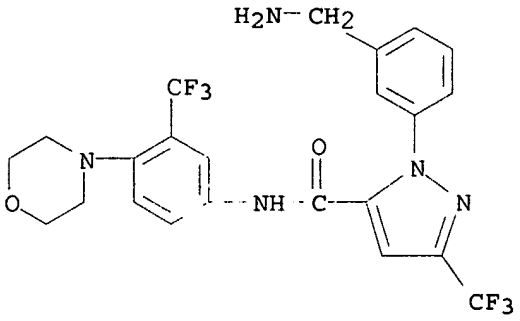
RN 209957-92-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-93-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

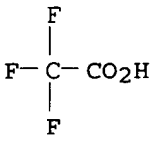
CM 1

CRN 209957-92-6
CMF C23 H21 F6 N5 O2

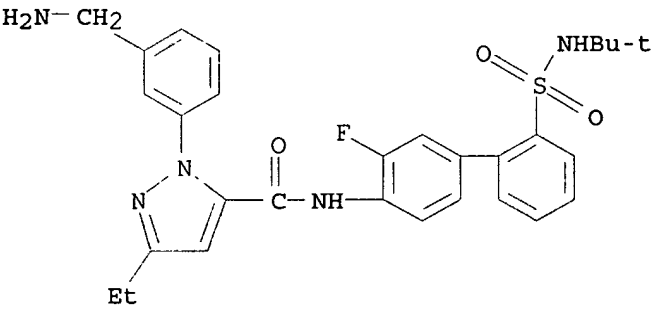


CM 2

CRN 76-05-1
CMF C2 H F3 O2



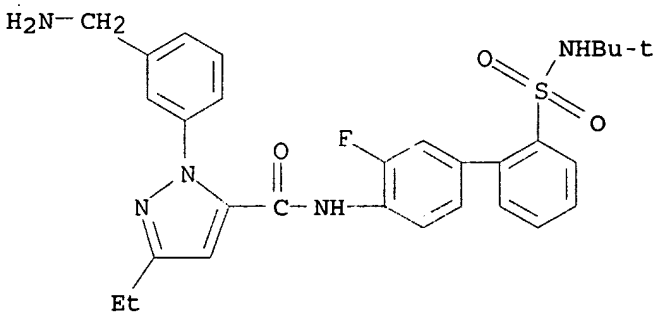
RN 209957-94-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-ethyl- (9CI) (CA INDEX NAME)



RN 209957-95-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-ethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

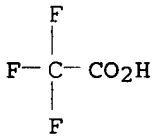
CM 1

CRN 209957-94-8
CMF C29 H32 F N5 O3 S

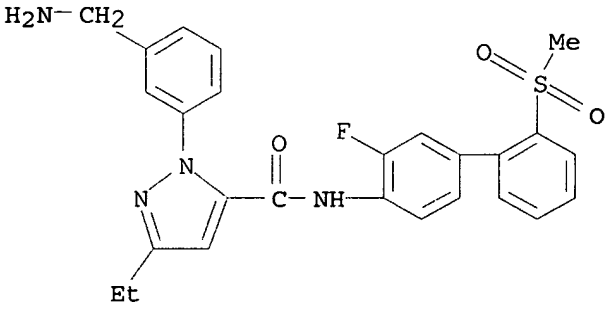


CM 2

CRN 76-05-1
CMF C2 H F3 O2



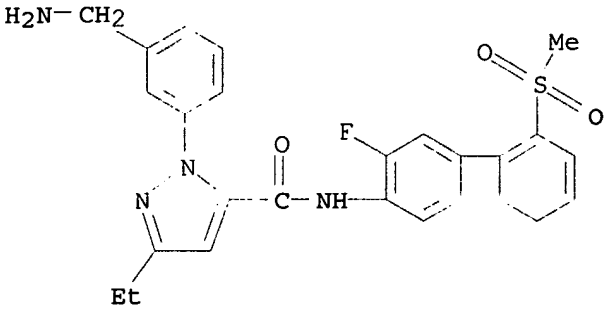
RN 209957-96-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-ethyl-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 209957-97-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-ethyl-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

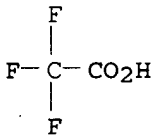
CM 1

CRN 209957-96-0
CMF C26 H25 F N4 O3 S

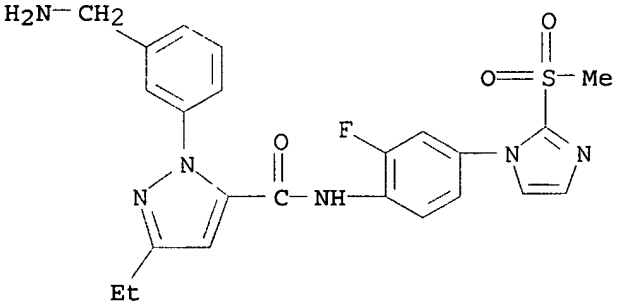


CM 2

CRN 76-05-1
CMF C2 H F3 O2



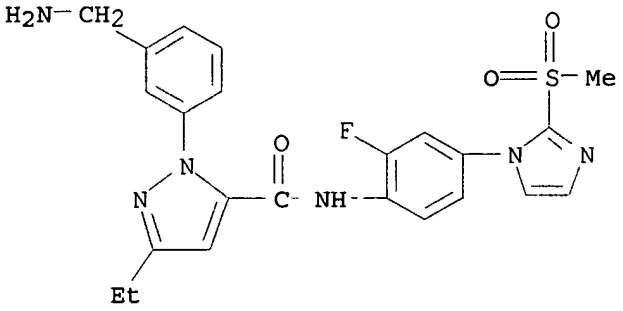
RN 209957-98-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-ethyl-N-[2-fluoro-4-[2-(methylsulfonyl)-1H-imidazol-1-yl]phenyl]- (9CI) (CA INDEX NAME)



RN 209957-99-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-3-ethyl-N-[2-fluoro-4-[2-(methylsulfonyl)-1H-imidazol-1-yl]phenyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

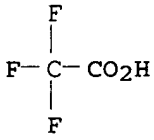
CM 1

CRN 209957-98-2
CMF C23 H23 F N6 O3 S

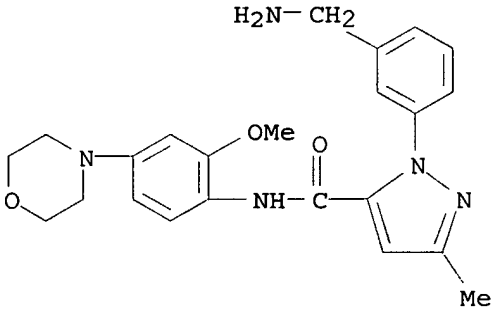


CM 2

CRN 76-05-1
CMF C2 H F3 O2



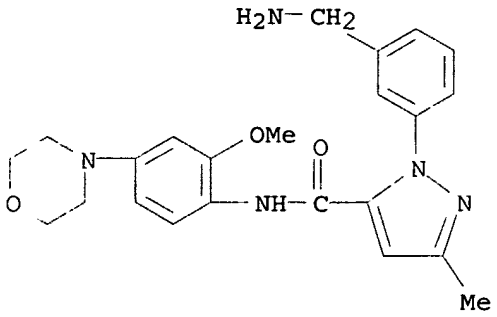
RN 209958-07-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-methoxy-4-(4-morpholinyl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209958-08-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-methoxy-4-(4-morpholinyl)phenyl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

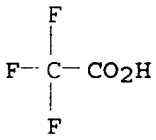
CM 1

CRN 209958-07-6
CMF C23 H27 N5 O3

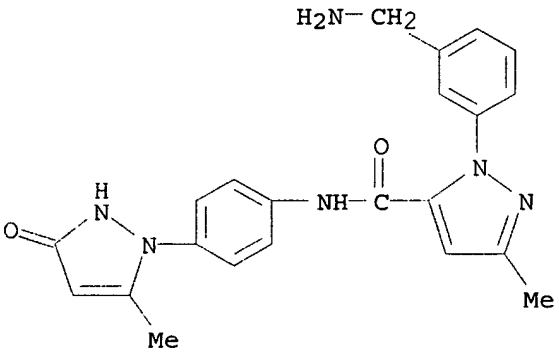


CM 2

CRN 76-05-1
CMF C2 H F3 O2



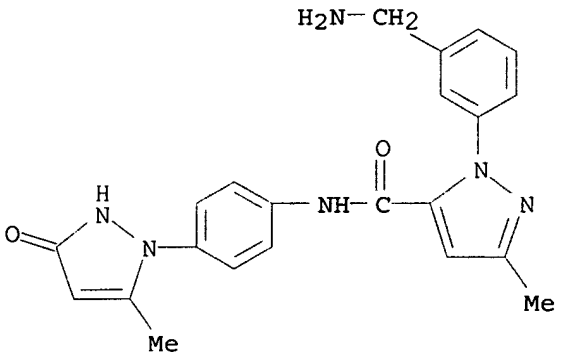
RN 209958-09-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209958-10-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

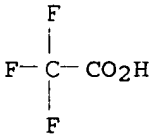
CM 1

CRN 209958-09-8
CMF C22 H22 N6 O2

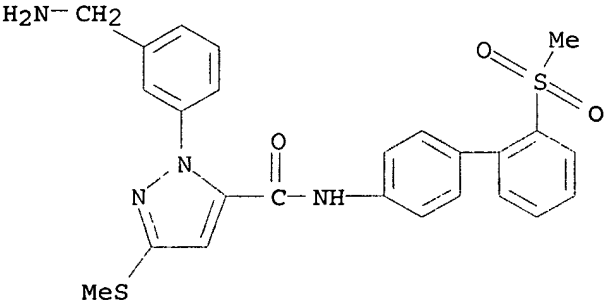


CM 2

CRN 76-05-1
CMF C2 H F3 O2



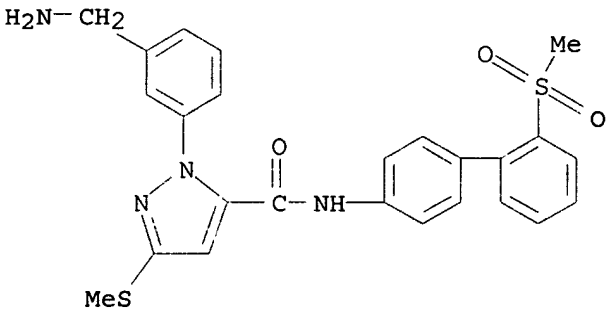
RN 209958-11-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylthio)- (9CI) (CA INDEX NAME)



RN 209958-12-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylthio)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

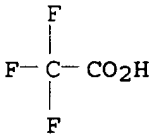
CM 1

CRN 209958-11-2
CMF C25 H24 N4 O3 S2

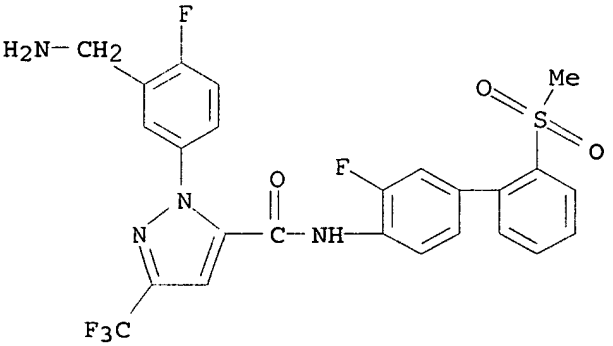


CM 2

CRN 76-05-1
CMF C2 H F3 O2



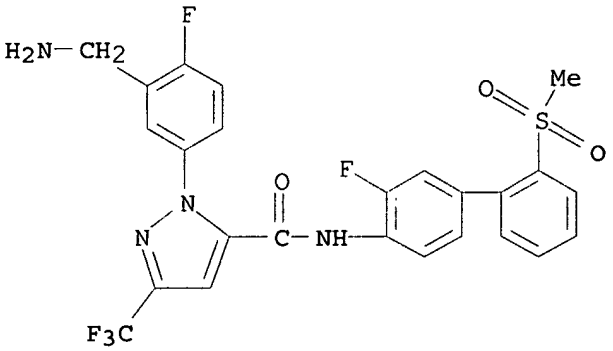
RN 209958-13-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209958-14-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

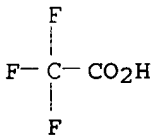
CM 1

CRN 209958-13-4
CMF C25 H19 F5 N4 O3 S

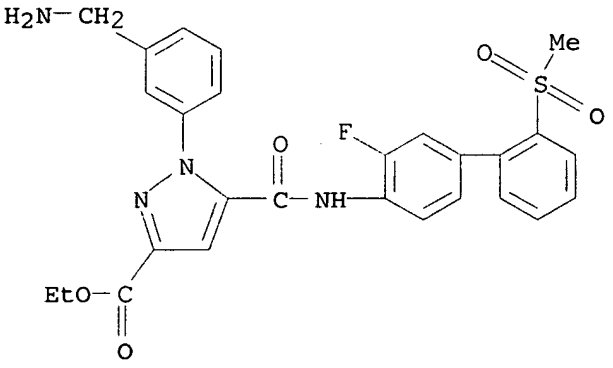


CM 2

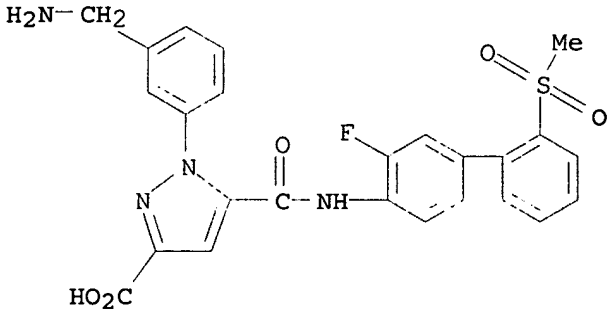
CRN 76-05-1
CMF C2 H F3 O2



RN 209958-15-6 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)



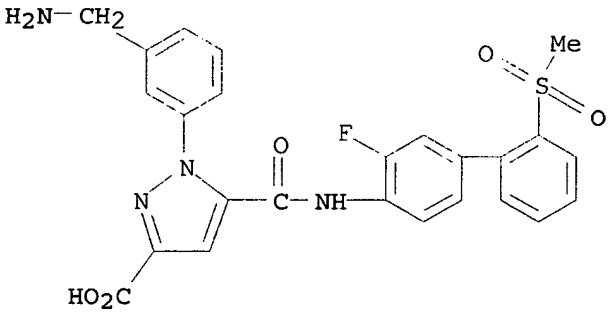
RN 209958-17-8 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)



RN 209958-18-9 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

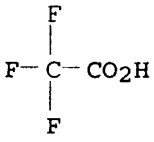
CM 1

CRN 209958-17-8
CMF C25 H21 F N4 O5 S

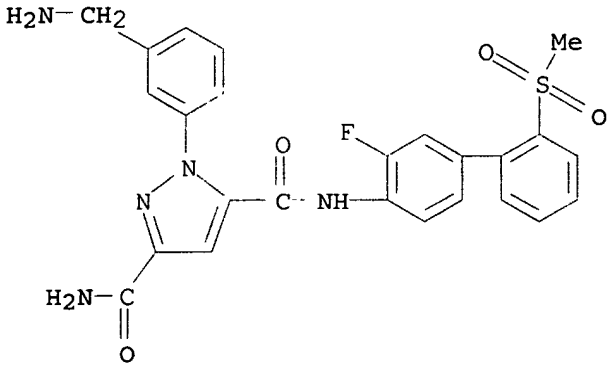


CM 2

CRN 76-05-1
CMF C2 H F3 O2



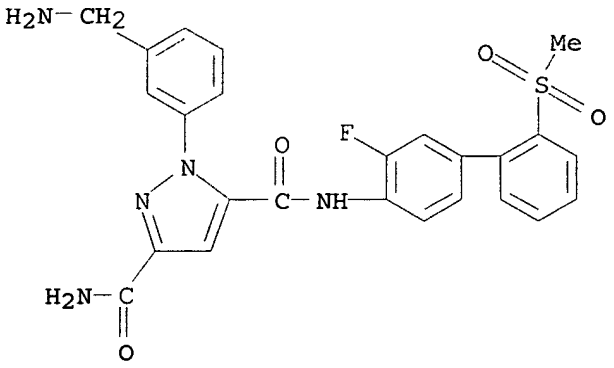
RN 209958-19-0 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxamide, 1-[3-(aminomethyl)phenyl]-N5-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 209958-20-3 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxamide, 1-[3-(aminomethyl)phenyl]-N5-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

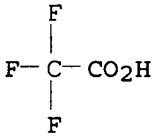
CM 1

CRN 209958-19-0
CMF C25 H22 F N5 O4 S

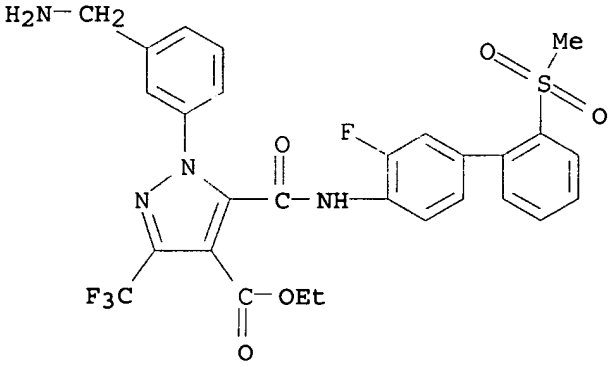


CM 2

CRN 76-05-1
CMF C2 H F3 O2



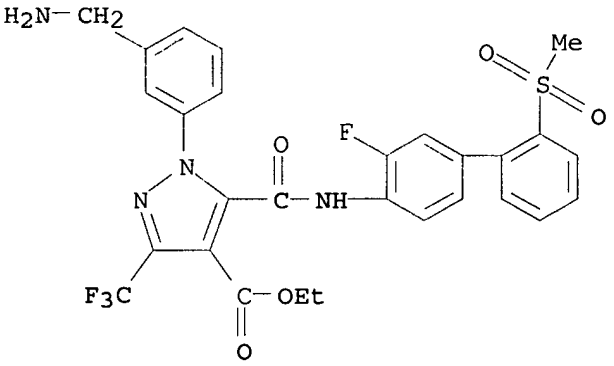
RN 209958-21-4 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 209958-22-5 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

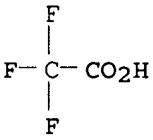
CM 1

CRN 209958-21-4
CMF C28 H24 F4 N4 O5 S



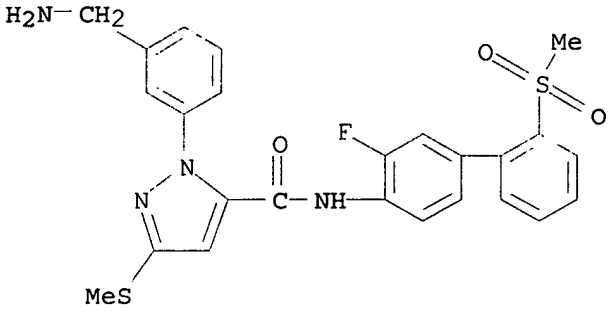
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 209958-24-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylthio)- (9CI) (CA INDEX

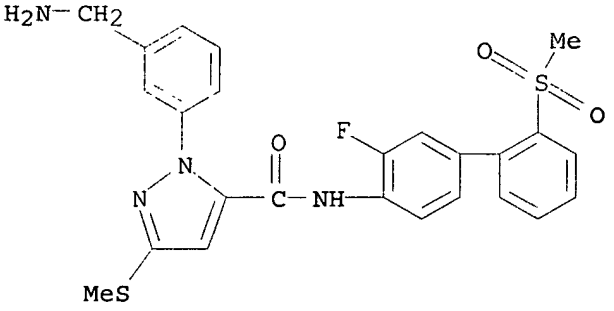
NAME)



RN 209958-25-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylthio)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

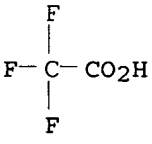
CM 1

CRN 209958-24-7
CMF C25 H23 F N4 O3 S2

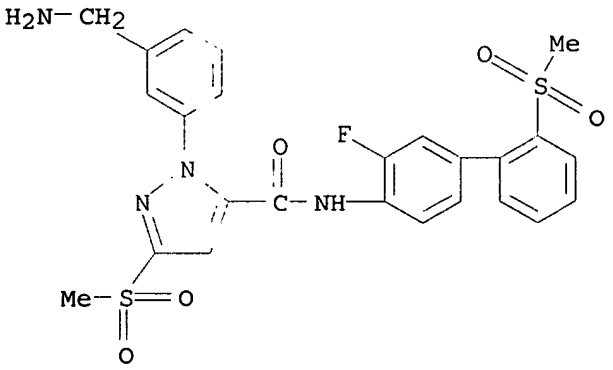


CM 2

CRN 76-05-1
CMF C2 H F3 O2



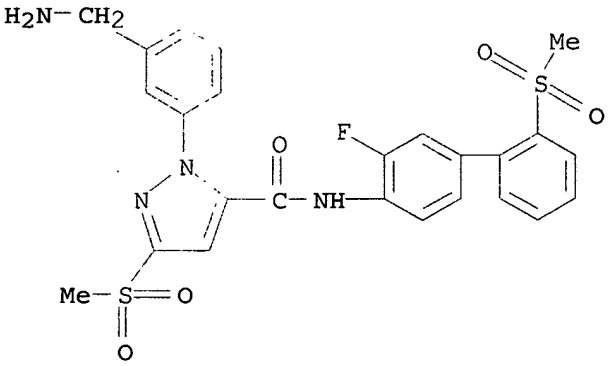
RN 209958-26-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylsulfonyl)- (9CI) (CA INDEX NAME)



RN 209958-27-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(methylsulfonyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-26-9
CMF C25 H23 F N4 O5 S2



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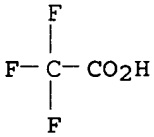
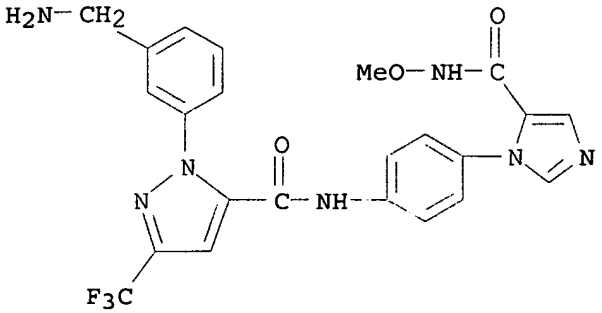
CRN 76-05-1
CMF C2 H F3 O2



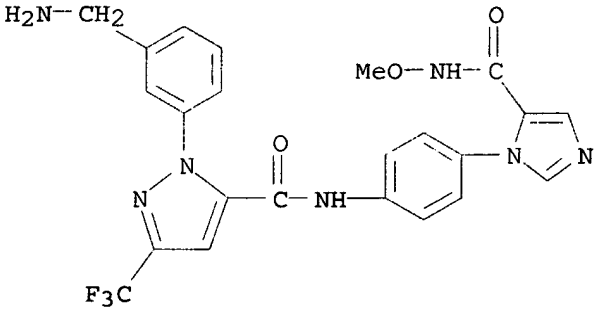
RN 209958-28-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-[(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209958-29-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-[(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-28-1
CMF C23 H20 F3 N7 O3



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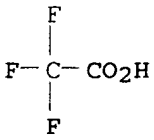
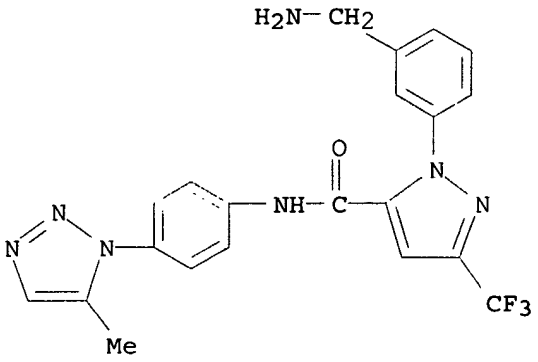


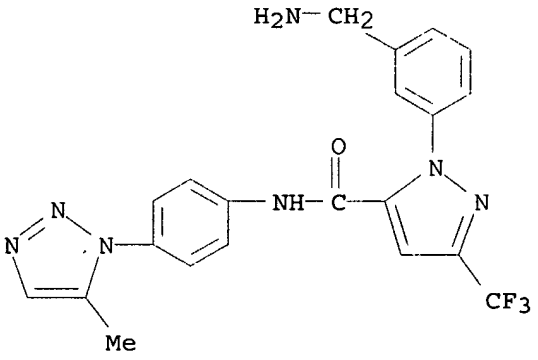
RN 209958-30-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209958-31-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

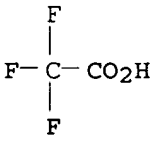
CM 1

CRN 209958-30-5
CMF C21 H18 F3 N7 O



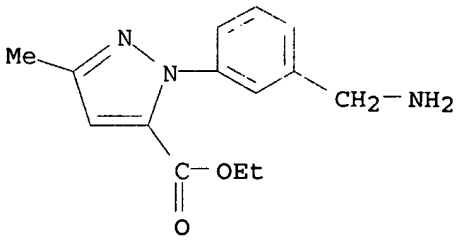
CM 2

CRN 76-05-1
CMF C2 H F3 O2



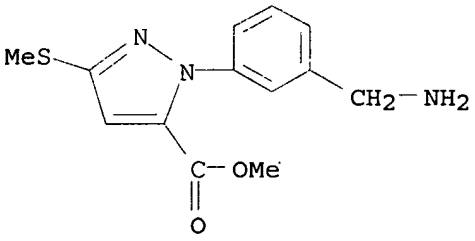
IT **209960-83-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors)
RN 209960-83-8 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 1-[3-(aminomethyl)phenyl]-3-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT **209960-51-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors)
RN 209960-51-0 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-[3-(aminomethyl)phenyl]-3-(methylthio)-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

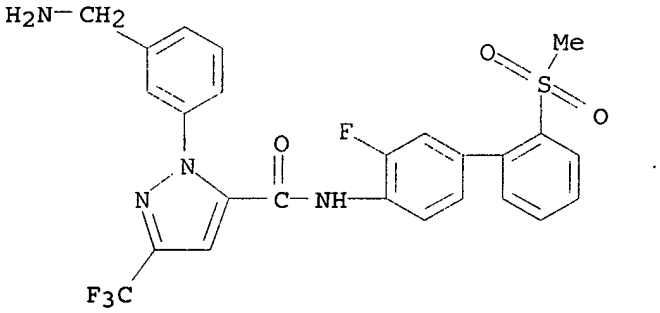
L7 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:777848 CAPLUS
TITLE: A Critical Assessment of Docking Programs and Scoring Functions
AUTHOR(S): Warren, Gregory L.; Andrews, C. Webster; Capelli, Anna-Maria; Clarke, Brian; LaLonde, Judith; Lambert, Millard H.; Lindvall, Mika; Nevins, Neysa; Semus, Simon F.; Senger, Stefan; Tedesco, Giovanna; Wall, Ian D.; Woolven, James M.; Peishoff, Catherine E.; Head, Martha S.
CORPORATE SOURCE: GlaxoSmithKline Pharmaceuticals, Collegeville, PA, 19426, USA
SOURCE: Journal of Medicinal Chemistry ACS ASAP
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Docking is a computational technique that samples conformations of small

mols. in protein binding sites; scoring functions are used to assess which of these conformations best complements the protein binding site. An evaluation of 10 docking programs and 37 scoring functions was conducted against eight proteins of seven protein types for three tasks: binding mode prediction, virtual screening for lead identification, and rank-ordering by affinity for lead optimization. All of the docking programs were able to generate ligand conformations similar to crystallog. determined protein/ligand complex structures for at least one of the targets. However, scoring functions were less successful at distinguishing the crystallog. conformation from the set of docked poses. Docking programs identified active compds. from a pharmaceutically relevant pool of decoy compds.; however, no single program performed well for all of the targets. For prediction of compound affinity, none of the docking programs or scoring functions made a useful prediction of ligand binding affinity.

IT **209957-47-1**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(critical assessment of docking programs and scoring functions)

RN 209957-47-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> cezanne/in
'IN' IS NOT A VALID FIELD CODE
L8 0 CEZANNE/IN

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	190.56	358.15
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
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STN INTERNATIONAL LOGOFF AT 12:51:20 ON 30 MAR 2006

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 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  DEC 23   New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/
                   USPAT2
 NEWS  4  JAN 13   IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
 NEWS  5  JAN 13   New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to
                   INPADOC
 NEWS  6  JAN 17   Pre-1988 INPI data added to MARPAT
 NEWS  7  JAN 17   IPC 8 in the WPI family of databases including WPIFV
 NEWS  8  JAN 30   Saved answer limit increased
 NEWS  9  FEB 21   STN AnaVist, Version 1.1, lets you share your STN AnaVist
                   visualization results
 NEWS 10  FEB 22   The IPC thesaurus added to additional patent databases on STN
 NEWS 11  FEB 22   Updates in EPFULL; IPC 8 enhancements added
 NEWS 12  FEB 27   New STN AnaVist pricing effective March 1, 2006
 NEWS 13  FEB 28   MEDLINE/LMEDLINE reload improves functionality
 NEWS 14  FEB 28   TOXCENTER reloaded with enhancements
 NEWS 15  FEB 28   REGISTRY/ZREGISTRY enhanced with more experimental spectral
                   property data
 NEWS 16  MAR 01   INSPEC reloaded and enhanced
 NEWS 17  MAR 03   Updates in PATDPA; addition of IPC 8 data without attributes
 NEWS 18  MAR 08   X.25 communication option no longer available after June 2006
 NEWS 19  MAR 22   EMBASE is now updated on a daily basis
 NEWS 20  APR 03   New IPC 8 fields and IPC thesaurus added to PATDPAFULL
 NEWS 21  APR 03   Bibliographic data updates resume; new IPC 8 fields and IPC
                   thesaurus added in PCTFULL
 NEWS 22  APR 04   STN AnaVist $500 visualization usage credit offered
 NEWS 23  APR 12   LINSPEC, learning database for INSPEC, reloaded and enhanced
 NEWS 24  APR 12   Improved structure highlighting in FQHIT and QHIT display
                   in MARPAT
 NEWS 25  APR 12   Derwent World Patents Index to be reloaded and enhanced during
                   second quarter; strategies may be affected

 NEWS EXPRESS  FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
               V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
               http://download.cas.org/express/v8.0-Discover/

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FILE 'HOME' ENTERED AT 08:34:50 ON 13 APR 2006

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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STRUCTURE FILE UPDATES: 11 APR 2006 HIGHEST RN 880129-32-8
DICTIONARY FILE UPDATES: 11 APR 2006 HIGHEST RN 880129-32-8

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****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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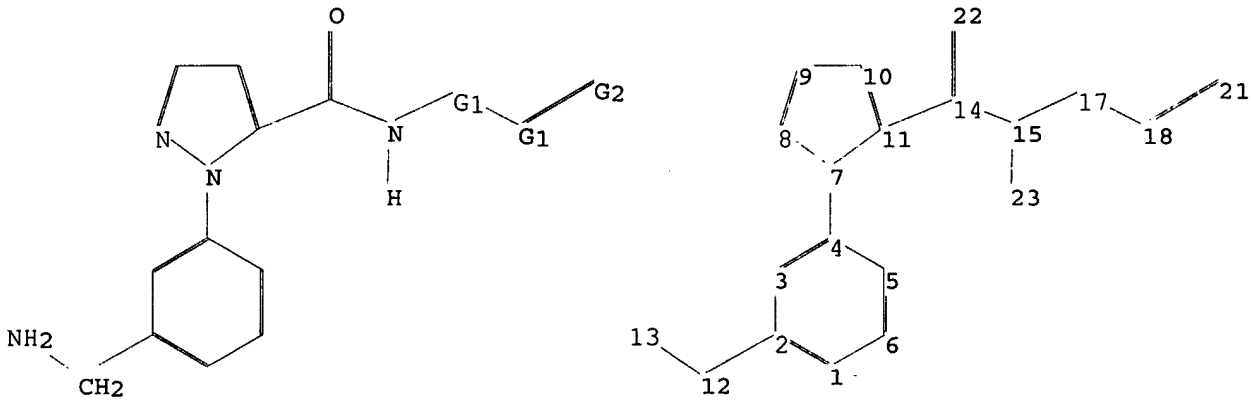
Uploading C:\Program Files\Stnexp\Queries\10519356\Struc 3.str



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ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
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ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
4-7 7-8 7-11 8-9 9-10 10-11 14-15 14-22 15-17 17-18 18-21
exact bonds :
2-12 11-14 12-13 15-23
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

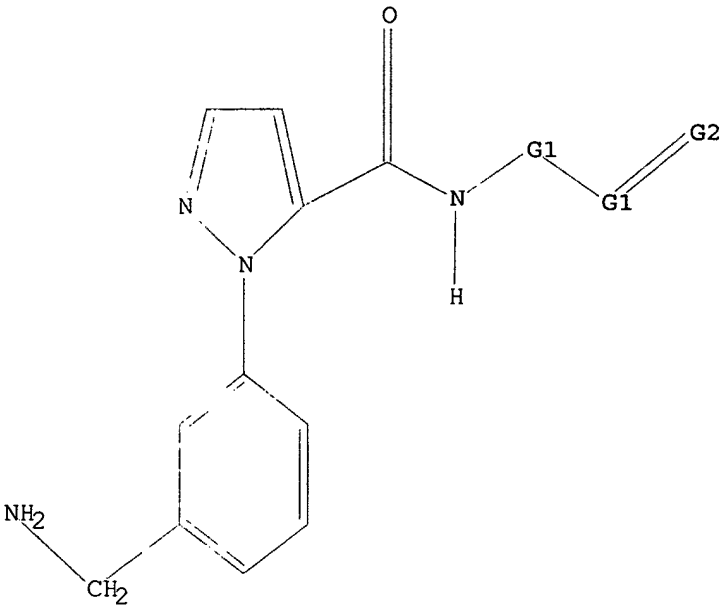
G1:Cb,Cy,Hy

G2:S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 21:CLASS
22:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 Cb,Cy,Hy

G2 S,N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -       46 TO ITERATE

100.0% PROCESSED       46 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          514 TO     1326
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

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FULL SCREEN SEARCH COMPLETED -      878 TO ITERATE

100.0% PROCESSED      878 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

L3            3 SEA SSS FUL L1

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   166.94     167.15

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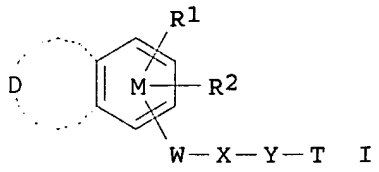
=> l3
L4 1 L3

=> d ibib abs hitstr

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:20490 CAPLUS
DOCUMENT NUMBER: 140:77148
TITLE: Preparation of N-[4-(thiooxoheterocyclyl)phenyl]-2-phenyl-2H-pyrazole-3-carboxamides and corresponding imino-heterocyclyl derivatives as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis
INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner; Tsaklakidis, Christos; Gleitz, Johannes; Barnes, Christopher
PATENT ASSIGNEE(S): Merck Patent Gmbh, Germany
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004002477	A1	20040108	WO 2003-EP5898	20030605
WO 2004002477	C1	20040415		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10229070	A1	20040115	DE 2002-10229070	20020628
CA 2491271	AA	20040108	CA 2003-2491271	20030605
AU 2003238475	A1	20040119	AU 2003-238475	20030605
EP 1517685	A1	20050330	EP 2003-732540	20030605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005535630	T2	20051124	JP 2004-516575	20030605
US 2005203127	A1	20050915	US 2004-519356	20041228
PRIORITY APPLN. INFO.:			DE 2002-10229070 A	20020628
			WO 2003-EP5898 W	20030605

OTHER SOURCE(S): MARPAT 140:77148
GI



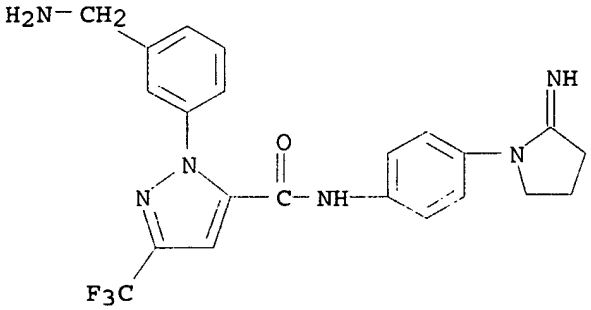
I

AB Title compds. [I; D = (N-, O-, S-interrupted) (substituted) C3-4 alkylene; M = Ph, aromatic heterocyclyl; R1, R2 = H, halo, (branched) (interrupted) (substituted) alkyl, NO2, cyano, OR3, N(R3)2, CO2R3, CON(R3)2, C(:S)N(R3)2, etc.; R3 = H, (branched) (interrupted) (substituted) alkyl, etc.; W = (substituted) (bi)cyclic aromatic (hetero)cyclyl; X = CONR3, CONR3C(R4)2, C(R4)2NR3, etc.; R4 = H, (branched) (interrupted) (substituted) alkyl; Y = alkylene, cycloalkylene, heterodiyl, aryldiyl; T = (substituted) (bi)cyclic aromatic heterocyclyl], were prepared Thus, 333 mg (3-[5-(4-[2-iminopyrrolidin-1-yl]phenylcarbamoyl)-3-trifluoromethylpyrazol-1-yl]benzyl)carbamic acid tert-Bu ester (preparation given) in EtOH was treated with HCl in ether to give 289 mg N-[4-(2-iminopyrrolidin-1-yl)phenyl]-1-(3-aminomethylphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide. The latter gave affinity to the receptor Xa with IC50 = 9,6·10-9 M and to the receptor VIIa with IC50 = 2,3·10-8 M.

IT **640287-97-4P 640288-21-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (thiooxoheterocyclylphenyl)(phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

RN 640287-97-4 CAPLUS

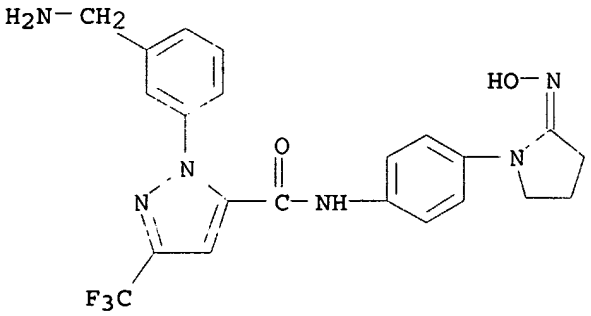
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 640288-21-7 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[2-(hydroxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.02	173.17

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.75	-0.75

STN INTERNATIONAL LOGOFF AT 08:35:55 ON 13 APR 2006